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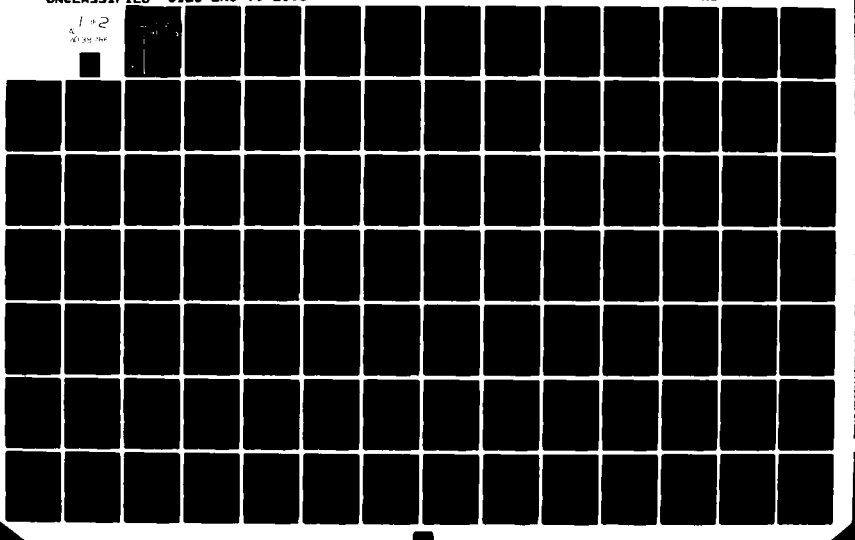

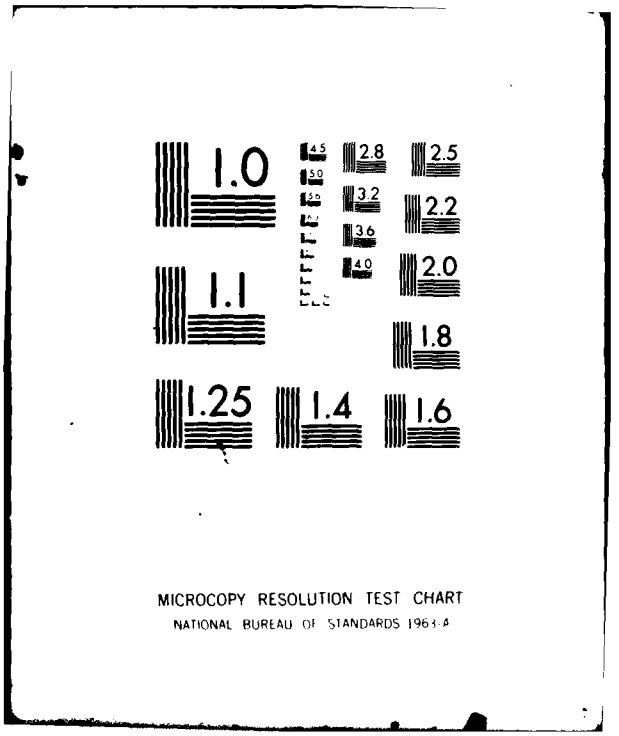
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SOLUTION TECHNIQUES FOR LARGE EIGENVALUE PROBLEMS IN STRUCTURAL DYNAMICS

LEVEL II

By
I.-W. LEE
A. R. ROBINSON

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16. Abstract (Limit: 200 words)

This study treats the determination of eigenvalues and eigenvectors of large algebraic systems. The methods developed are applicable to finding the natural frequencies and modes of vibration of large structural systems.

For distinct eigenvalues the method is an application of the modified Newton-Raphson method that turns out to be more efficient than the standard competing schemes.

For close or multiple eigenvalues, the modified Newton-Raphson method is generalized to form a new process. The entire set of close eigenvalues and their eigenvectors are found at the same time in a two-step procedure. The subspace of the approximate eigenvectors is first projected onto the subspace of the true eigenvectors. If the eigenvalues are multiple, the results of the first stage indicate this fact and the process terminates. If they are merely close, a single rotation in the newly found space solves a small eigenvalue problem and provides the final results for the close set. The procedure for subspace projection can be expressed as a simple extremum problem that generalizes the known extremum property of eigenvectors.

Computational effort and convergence are studied in three example problems. The method turns out to be more efficient than subspace iteration.

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1. INTRODUCTION

1.1 General

Various engineering problems can be reduced to the solution of matrix eigenvalue problems. Typical examples in the field of structural engineering are the problem of determination of natural frequencies and the corresponding normal modes in a dynamic analysis and the problem of finding buckling loads in a stability analysis of structures. Since the advent of the digital computer, the complexity of structures which can be treated and the order of the corresponding eigenvalue problems have been greatly increased. Hence, the development of solution techniques for such problems has attracted much attention.

For the dynamic analysis of a linear discrete structural system by superposition of modes, we must first solve the problem of free vibration of the system. The free vibration analysis of the linear system without damping reduces to the solution of the linear eigenvalue problem

$$A\bar{x} = \lambda B\bar{x} \tag{1.1}$$

in which A and B are stiffness and mass matrices of order n, the number of degrees of freedom of the structural system. A column vector $\bar{x}$ is an eigenvector (or normal mode), and the scalar λ the corresponding eigenvalue (or the square of a natural frequency).

The matrices A and B are real and symmetric, and are usually banded and sparse. If a consistent mass matrix is used, the matrices A and B have the

same bandwidth [4,5]. If a lumped mass model of the system is used, B will be diagonal. The matrix B is positive definite, but the matrix A may be semidefinite. There are n sets of solutions of Eq. (1.1), that is, n eigenvalues and their corresponding eigenvectors.

Frequently, in practical eigenvalue problems, the order of A and B is so high that it is impractical or very expensive to obtain the complete eigensolution. On the other hand, to carry out a reasonably accurate dynamic analysis of the structure, it is possible to consider only a partial eigensolution. The partial solution of interest may consist of only few lowest eigenvalues and their eigenvectors, or eigenvalues in the vicinity of a given frequency and the corresponding eigenvectors. The method described in this study is aimed at effective solution of this type of problem rather than at a complete eigensolution.

1.2 Object and Scope

The object of this study is to present an iterative method which is efficient and numerically stable for the accurate computation of limited number of eigenvalues and the corresponding eigenvectors of linear eigenvalue problems of large order.

The method developed remedies the major drawbacks of the inverse iteration method with spectral shifting [13]: numerical instability due to shifting and slow convergence when eigenvalues are equal or close in magnitude. The proposed method converges rapidly and is numerically stable for any number of multiple or close eigenvalues and the corresponding eigenvectors.

The procedure for distinct eigenvalues is treated in Chapter 2, and a modified procedure for multiple or close eigenvalues in Chapter 3. Selection of initial approximate eigenvalues and eigenvectors by the subspace iteration method is described in Chapter 4. To show the efficiency of the proposed method, three sample problems are solved: vibration of a plane frame, of a plate in bending, and of an arch. Comparisons are made in Chapter 5 with a method which is generally regarded as very efficient, the subspace iteration method.

1.3 Review of Solution Methods

Numerous techniques for the solution of eigenvalue problems have been developed. These techniques can be divided into two classes - techniques for approximate solution and techniques for "exact" solution.

The approximate solution techniques include well-known static condensation [2,3,24,25,27,42], dynamic condensation [34], Rayleigh-Ritz analysis [9,13,31,48], component mode analysis and related methods summarized by Uhrig [50]. These methods are essentially techniques for reducing the size of a system of equations. The reduction of a system of equations eventually leads to a loss in accuracy of a solution. However, the advantage of lessened computational effort for a solution sometimes may compensate for the loss in accuracy. Moreover, an approximate solution found by these methods may serve as the starting solution for the exact methods, which will be discussed next.

The exact methods are designed for the accurate computation of some or all the eigenvalues and corresponding eigenvectors. These methods consist

of vector iteration methods, transformation methods, the method based on the Sturm-sequence property, polynomial iteration method, and minimization methods. These methods are well described in Ref. 51. The methods differ in the choice of which mathematical properties of an eigenvalue problem are used. The vector iteration methods such as the classical vector iteration (power method) and simultaneous vector iteration deal with the form of equations $A\bar{x} = \lambda B\bar{x}$. The transformation methods (LR, QR, Jacobi, Givens, and Householder methods) are based on the mathematical property that the eigenvalues of a system are invariant under similarity transformations. In the polynomial iteration method, the roots of $\det (A - \lambda B) = 0$ are found, and minimization methods are based on the stationary property of the Rayleigh quotient [43].

In vector iteration methods and minimization methods, both the eigenvalues and corresponding eigenvectors are found simultaneously, but in other exact methods, only eigenvalues are computed or the computed eigenvectors are, in general, not suitable for use in the final solutions. In such methods, another method such as the vector iteration method with a shift may be used for finding the eigenvector corresponding to a computed eigenvalue.

For a limited number of eigenvalues and corresponding eigenvectors of an eigenvalue problem of large order which we are concerned with in this study, the above methods have been modified or combined to take advantage of the useful characteristics of several of the methods. First, the determinant search method [7,9,22,23] combines the methods based on the Sturm-sequence property, polynomial iteration, and inverse iteration. In this

method, eigenvalues in a specified range are approximately isolated by using the bisection method and the Sturm-sequence property and then located accurately by the polynomial iteration method. The corresponding eigenvectors are computed by inverse iteration with a shift. By this method, eigenvalues in any range and corresponding eigenvectors can be found. However, it has the disadvantage that the matrix is factorized in each iteration to locate the eigenvalues of interest.

Another method for the solution of large eigenvalue problems is the so-called subspace iteration method [6,15,32,39,47], which is a combination of the simultaneous iteration method and a Rayleigh-Ritz analysis. In this method, several independent vectors are improved by vector inverse iteration, and the best approximation to the eigenvectors are found in the subspace of the iteration vectors by a Rayleigh-Ritz analysis. In this method, eigenvalues at the end of the spectrum and the corresponding eigenvectors converge very rapidly. This method will be discussed further in Chapter 4.

The inverse iteration method with a shift is known to be extremely efficient for improving approximate eigenvalues and eigenvectors. However, as mentioned in the previous section, when the shift is very close to a true eigenvalue, the method exhibits numerical instability, yielding unreliable answers [13]. In addition, when the eigenvalues of interest are close together, their convergence is very slow. Robinson and Harris [44] developed an efficient method to overcome the above difficulty for distinct eigenvalues by augmenting the equations used in the inverse iteration method by a side equation. While this method extracts eigenvalues and eigenvectors simultaneously with a very high convergence rate, it has the disadvantage that the

algorithm is inefficient for problems with multiple or close eigenvalues. This method and some improvements on it will be discussed further in the next chapter.

1.4 Notation

All symbols are defined in the text when they first appear.

With regard to matrices, vectors, elements of matrices or vectors, and iteration steps, the following conventions are generally used:

(1) Matrices are denoted by uppercase letters, as A, B and X.

(2) A column vector is denoted by a lowercase letter with a superior bar and a subscript, as $\bar{a}_j$, $\bar{b}_j$ and $\bar{x}_j$.

(3) Elements of a matrix or vector are denoted by a lowercase letter with a double subscripts, as a_{ij}, b_{ij} and x_{ij}.

(4) Iteration steps are denoted by a superscript, as $X^{(k)}$, $\bar{x}_j^{(k)}$ and $x_{ij}^{(k)}$.

(5) Increments are denoted by the symbol Δ, as $\Delta x_j^{(k)}$ and $\Delta x_{ij}^{(k)}$.

Some symbols are assigned more than one meaning. However, in the context of their use there are no ambiguities.

A, $\bar{a}_j$, $\bar{a}_{ij}$ = stiffness matrix, j^{th} column vector of A, element of A

$A^{*(k)}$ = projection of A onto the subspace spanned by vectors in $Y^{(k)}$, $A^{*(k)} = Y^{(k)T} A Y^{(k)}$

a = radius of circular arch

B, $\bar{b}_j$, b_{ij} = mass matrix, j^{th} column vector of B, element of B

$B^{*(k)}$ = projection of B onto the subspace spanned by vectors in $Y^{(k)}$, $B^{*(k)} = Y^{(k)T} B Y^{(k)}$

$C^{(k)}$, $\bar{c}_j^{(k)}$, $c_{ij}^{(k)}$ = expansion matrix of $X^{(k)}$, j^{th} column vector of $C^{(k)}$, element of $C^{(k)}$, $X^{(k)} = XC^{(k)}$

D = diagonal matrix, see Section 2.2

D_e = plate bending stiffness, $D_e = EH^3/12(1-\upsilon^2)$

D, $\bar{d}_j$ = matrix for finding close or multiple eigenvalues and eigenvectors, jth column vector of D, see Eq. (3.24)

$D^{(k)}$, $\bar{d}_j^{(k)}$ = iteration matrix for D after k iterations, jth column vector of $D^{(k)}$, see Eq. (3.23)

E = Young's modulus

E, $\bar{e}_j$, e_{jj} = diagonal matrix, jth column vector of E, element of E, see Eq. (A.7)

E^*, $\bar{e}_j^*$, $\bar{e}_{jj}^*$ = diagonal matrix, jth column vector of E^*, element of E^*, $E^* = -E^{-1}$

h = thickness of plate

= number indicating rate of convergence of eigenvector, see Eq. (2.13)

I = moment of inertia of cross-section

I_s = identity matrix of order s

i, j = indices of matrix elements

k = superscript indicating number of iterations

L = lower triangular matrix

= Lagrangian, see Eq. (3.6)

m_a, m_b = average half bandwidth of A, of B

N_p, N_r, N_s = total number of operations required for finding eigenpairs by the proposed method, by the Robinson-Harris method, by the subspace-iteration method

n = order of A and B

p = number of eigenpairs sought

q = number of iteration vectors by subspace iteration method, $q = \max(2p, p+8)$

$\bar{r}_j^{(k)}$ = residual vector of approximation to jth eigenpair after k iterations

s = number of close and/or multiple eigenpairs sought

T_p, T_r, T_s = number of iterations needed to find eigenpairs by proposed method, by Robinson-Harris method, by subspace iteration method

$X, \bar{x}_j, x_{ij}$ = matrix of eigenvectors (modal matrix), jth eigenvector, element of X

$X^{(k)}, \bar{x}_j^{(k)}, x_{ij}^{(k)}$ = approximation to X after k iterations, jth column vector of $X^{(k)}$, element of $X^{(k)}$

$Y^{(k)}, \bar{y}_j^{(k)}, y_{ij}^{(k)}$ = matrix of iteration vectors improved from $X^{(k)}$ by simultaneous iteration method, jth column vector of $Y^{(k)}$, element of $Y^{(k)}$

$Z, Z^{(k)}$ = rotation matrix, approximation to Z after k iterations

$\gamma_j^{(k)}$ = error in $\lambda_j^{(k)}$ or $\mu_{jj}^{(k)}$

Δ = increment operator

δ_{ij} = Kronecker delta

$\theta_j^{(k)}$ = error in $\bar{x}_j^{(k)}$ or $\bar{y}_j^{(k)}$

λ^* = multiple eigenvalue

Λ, λ_j = diagonal matrix of eigenvalues, jth eigenvalue, $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_s)$

$\Lambda^{(k)}$, $\lambda_j^{(k)}$ = approximation to Λ, to λ_j, after k iterations

μ = shift applied in vector iteration method

μ_{ij}, $\mu_{ij}^{(k)}$ = element of D, of $D^{(k)}$

ρ = mass density

ω = natural circular frequency, $\lambda = \omega^2$

2. DISTINCT ROOTS

2.1 General

In this chapter, a method for finding a simple eigenvalue and the corresponding eigenvector will be presented. The method developed by Robinson and Harris [44] is modified here to save overall computational effort for finding an eigensolution. The Robinson-Harris method is an application of the Newton-Raphson technique for improving the accuracy of an approximate eigenvalue and the corresponding approximate eigenvector. In the proposed method, a modified form of the Newton-Raphson technique is applied instead of the standard one used in the Robinson-Harris method.

In Section 2.2, the Robinson-Harris method will be discussed first; then the proposed method will be presented. The convergence rate of the proposed method and the number of operations per iteration will be given in Section 2.3. The estimation of error in an approximate solution is found in Section 2.4. A technique for the examination of the converged solution to determine whether the eigenvalues and corresponding eigenvectors of interest have been missed and a method for finding a missed solution will be presented in Section 2.5.

2.2 The Iterative Scheme

Let us consider the following linear eigenvalue problem

$$A\bar{x}_j = \lambda_j B\bar{x}_j \qquad (j = 1, 2, \ldots, n) \qquad (2.1)$$

where A and B are assumed to be given symmetric matrices of order n and B is taken to be positive definite. The λ_j and $\bar{x}_j$ are the jth eigenvalue and the corresponding eigenvector.

Let us assume that an initial approximate solution of Eq. (2.1), $\lambda_j^{(0)}$ and $\bar{x}_j^{(0)}$, is available. Denote an approximate eigenvalue and the corresponding eigenvector after k iterations by $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$ (k = 0, 1, . . .). Then, we have

$$A\bar{x}_j^{(k)} - \lambda_j^{(k)} B\bar{x}_j^{(k)} = \bar{r}_j^{(k)} \tag{2.2}$$

where $\bar{r}_j^{(k)}$ is a residual vector.

The object is to remove the residual vector in Eq. (2.2). The Newton-Raphson technique is applied for this purpose. Let the (k + 1)th approximation be defined by

$$\begin{aligned} \lambda_j^{(k+1)} &= \lambda_j^{(k)} + \Delta\lambda_j^{(k)} \\ \bar{x}_j^{(k+1)} &= \bar{x}_j^{(k)} + \Delta\bar{x}_j^{(k)} \end{aligned} \tag{2.3}$$

where $\Delta\lambda_j^{(k)}$ and $\Delta\bar{x}_j^{(k)}$ are small unknown incremental changes of $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$. Substituting $\lambda_j^{(k+1)}$ and $\bar{x}_j^{(k+1)}$ of Eq. (2.3) for λ_j and $\bar{x}_j$ in Eq. (2.1) and discarding a nonlinear term $\Delta\lambda_j^{(k)} \cdot B\Delta\bar{x}_j^{(k)}$ as very small compared with the other, linear, terms, we get

$$(A - \lambda_j^{(k)} B)\,\Delta\bar{x}_j^{(k)} - \Delta\lambda_j^{(k)} B\bar{x}_j^{(k)} = -\bar{r}_j^{(k)} \tag{2.4}$$

where $\bar{r}_j^{(k)}$ is the residual vector defined in Eq. (2.2).

Note that in Eq. (2.4), there are n+1 scalar unknowns ($\Delta\lambda_j^{(k)}$ and n components of $\Delta\bar{x}_j^{(k)}$), but only n equations. Hence, it is required for the solution of Eq. (2.4) that either the number of unknowns be reduced or one equation added. Derwidue [16] and Rall [41] reduced the number of unknowns by setting the nth component of the vector $\Delta\bar{x}_j^{(k)}$ or $\bar{x}_j^{(k+1)}$ at a preassigned value - zero or one. In these methods, it may happen that an unfortunate choice of one component results in failure of the procedure.

Instead of reducing the number of unknowns, Robinson and Harris [44] added an extra equation (side condition) to the system of Eq. (2.4), to arrive at a set of n+1 equations in n+1 unknowns. This side condition is

$$\bar{x}_j^{(k)T} B\Delta\bar{x}_j^{(k)} = 0 \tag{2.5}$$

Equation (2.5) means that the incremental value $\Delta\bar{x}_j^{(k)}$ is orthogonal to the current approximate eigenvector $\bar{x}_j^{(k)}$ with respect to the matrix B. The side condition prevents unlimited change in the $\bar{x}_j^{(k)}$. The resulting set of simultaneous linear equations may be written in matrix form as

$$\begin{bmatrix} A - \lambda_j^{(k)}B & -B\bar{x}_j^{(k)} \\ -\bar{x}_j^{(k)T}B & 0 \end{bmatrix} \begin{bmatrix} \Delta\bar{x}_j^{(k)} \\ \Delta\lambda_j^{(k)} \end{bmatrix} = \begin{bmatrix} -\bar{r}_j^{(k)} \\ 0 \end{bmatrix} \tag{2.6}$$

where the residual vector $\bar{r}_j^{(k)}$ is given in Eq. (2.2). The coefficient matrix for the incremental values is of order n+1 and symmetric. Moreover, it is nonsingular if λ_j is not multiple [44]. Equation (2.6) may be solved for $\Delta\lambda_j^{(k)}$ and $\Delta\bar{x}_j^{(k)}$ by Gauss elimination, or by any other suitable

technique. Note that the submatrix in the coefficient matrix $(A - \lambda_j^{(k)}B)$ is almost singular when $\lambda_j^{(k)}$ is close to λ_j. However, this does not cause any difficulty in solving Eq. (2.6), since in the elimination process only the last pivot element, in general, becomes very small. Thus, the interchange of columns and rows does not increase significantly the column height of the factorized matrix. The improved values, $\lambda_j^{(k+1)}$ and $\bar{x}_j^{(k+1)}$, are computed from Eq. (2.3). The procedure employing Eqs. (2.3) and (2.6) is repeated until the errors in the $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$ are within allowable tolerances. The method of estimating these errors will be discussed in Section 2.4.

The convergence of the above process for an eigenvalue and the corresponding eigenvector has been shown to be better than second order; the order has been found to be 2.41 [44]. However, the algorithm using Eq. (2.6) requires a new triangularization in each iteration, since the values of the elements of the coefficient matrix are changed in each iteration as a result of changing from $\lambda_j^{(k)}$ to $\lambda_j^{(k+1)}$. The number of operations (multiplications and divisions) required in such a triangularization is very large.

To avoid the complete elimination procedure in each iteration, the following equations instead of Eq. (2.6) are used in the proposed method.

$$\begin{bmatrix} A - \lambda_j^{(0)}B & -B\bar{x}_j^{(k)} \\ -\bar{x}_j^{(k)T}B & 0 \end{bmatrix} \begin{bmatrix} \Delta\bar{x}_j^{(k)} \\ \Delta\lambda_j^{(k)} \end{bmatrix} = \begin{bmatrix} -\bar{r}_j^{(k)} \\ 0 \end{bmatrix} \qquad (2.7)$$

where the residual vector $\bar{r}_j^{(k)}$ is defined in Eq. (2.2). Equation (2.7) was obtained by introducing Eq. (2.3) into Eq. (2.1) and discarding a small linear term $(\lambda_j^{(k+1)} - \lambda_j^{(0)})\, B\Delta\bar{x}_j^{(k)}$. Note that Eq. (2.7) differs from Eq. (2.6) in such a way that the coefficient matrix in Eq. (2.6) has the submatrix $(A - \lambda_j^{(k)}B)$, while the coefficient matrix in Eq. (2.7) has $(A - \lambda_j^{(0)}B)$. The coefficient matrix in Eq. (2.7) is also symmetric, and nonsingular if λ_j is not multiple. The nonsingularity of the coefficient matrix will be proved, in passing, in Appendix A.

From the form of the coefficient matrix, it can be seen that once the matrix is decomposed into the form LDL^T, where L is lower triangular and D is diagonal, only a small number of additional operations is required for the solution of Eq. (2.7) in the succeeding iterations, since only the vector $B\bar{x}_j^{(k)}$ in the matrix is changed in each iteration. The proposed method therefore considerably reduces the number of operations required in each iteration. On the other hand, the method lowers the convergence rate because of the neglect of the small linear term $(\lambda_j^{(k+1)} - \lambda_j^{(0)})\, (B\Delta x_j^{(k)})$, which in turn increases the number of iterations for a solution. However, the overall computational effort for a solution does decrease. It will be seen in Chapter 5 that the proposed method is actually more efficient than the Robinson-Harris method.

2.3 Convergence Rate and Operation Count

The efficiency of a numerical method such as the one proposed here can be estimated given the convergence rate and the number of operations per iteration required in the process. The convergence analysis, which is given

in Appendix B, will be summarized as follows. Let an approximate eigenvector $\bar{x}_j^{(k)}$ be expanded in terms of the true eigenvectors $\bar{x}_i$, i.e.,

$$\bar{x}_j^{(k)} = \sum_{i=1}^{n} c_{ij}^{(k)} \bar{x}_i \tag{2.8}$$

where $c_{ij}^{(k)}$ is a coefficient of the vector $\bar{x}_i$. If $\gamma_j^{(k)}$ is the error in $\lambda_j^{(k)}$ and $\theta_j^{(k)}$ the error in $\bar{x}_j^{(k)}$, they may be defined as

$$\gamma_j^{(k)} = \left| \frac{\lambda_j - \lambda_j^{(k)}}{\lambda_j} \right| \tag{2.9}$$

$$\theta_j^{(k)} = \left[\frac{\sum_{\substack{i=1 \\ i \neq j}}^{n} (c_{ij}^{(k)})^2}{\sum_{i=1}^{n} (c_{ij}^{(k)})^2} \right]^{1/2} \tag{2.10}$$

where $\theta_j^{(k)}$ is a measure of the angle between the vectors $\bar{c}_j^{(k)}$ and $\bar{c}_j$, and where $\bar{c}_j^{(k)T} = (c_{1j}^{(k)}, c_{2j}^{(k)}, \ldots, c_{nj}^{(k)}$ and $\bar{c}_j^T = (0,..,0, c_{jj}^{(k)}, 0, \ldots, 0)$. The geometric interpretation of $\theta_j^{(k)}$ is illustrated in Fig. 1.

With the above definitions, the errors in $\lambda_j^{(k+1)}$ and $\bar{x}_j^{(k+1)}$ may be written as (see Appendix B)

$$\gamma_j^{(k+1)} = h^2 \gamma_j^{(k)} \tag{2.11}$$

$$\theta_j^{(k+1)} = h\theta_j^{(k)} \tag{2.12}$$

where

$$h = \max_{m \neq j} \left| \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_m - \lambda_j^{(0)}} \right| \leq 1 \quad (m = 1, 2, \ldots n) \tag{2.13}$$

Equations (2.11) and (2.12) show that the convergence character of both eigenvalues and eigenvectors is linear. However, the eigenvalues converge much more rapidly than the eigenvectors. Note also that the closer λ_j is to another eigenvalue, the larger α is, yielding slow convergence. Hence, the method is not suitable for finding close eigenvalues and the corresponding eigenvectors.

Another important consideration which should be taken into account in estimating the efficiency of numerical methods is the number of operations per iteration. One operation is defined as one multiplication or division, which almost always is followed by an addition or a subtraction. For the expression of this number, let m_a and m_b be the half band-widths of the matrices A and B, and let n be the order of A and B. Let T_p be the number of iterations needed to find p eigenpairs by the proposed method and T_r by the Robinson-Harris method. Then, the number of operations for p eigenpairs, N_p, required by the proposed method is

$$N_p = \frac{1}{2}pn\,(m_a^2 + 3m_a + 2m_b + 2) + T_p n\,(5m_a + 2m_b + 6) \tag{2.14}$$

and by the Robinson-Harris method, N_r, is

$$N_r = \frac{1}{2} T_r n \, (m_a^2 + 13m_a + 6m_b + 12) \tag{2.15}$$

It can be seen that the number of operations per iteration required by the proposed method is much smaller than for the Robinson-Harris method. The development of the above expressions is given in Table 1.

2.4 Errors in Approximate Eigensolutions

An important feature of an iterative method such as the proposed method is some means of estimating the error in a computed solution. This permits one to terminate the iteration process at the point where a sufficiently accurate result has been obtained. It is important to have estimates in terms of numbers available in the calculation, since it is impossible to compare with the exact values.

The error in $\lambda_j^{(k)}$, $\gamma_j^{(k)}$, can be estimated as follows: from Eqs. (2.9) and (2.11)

$$\lambda_j = \lambda_j^{(k+1)} \pm h^2 \gamma_j^{(k)} \lambda_j \tag{2.16}$$

Substituting Eq. (2.16) for λ_j in Eq. (2.9) gives

$$\gamma_j^{(k)} = \left| 1 - \frac{\lambda_j^{(k)}}{\lambda_j} \right|$$

$$= \left| 1 - \frac{\lambda_j^{(k)}}{\lambda_j^{(k+1)} \left[1 \pm h^2 \gamma^{(k)} \lambda_j / \lambda_j^{(k+1)}\right]} \right| \tag{2.17}$$

Since $0 < h << 1$ and $0 \leq \gamma_j^{(k)} << 1$, from Eq. (2.17)

$$\gamma_j^{(k)} \simeq \left| 1 - \frac{\lambda_j^{(k)}}{\lambda^{(k+1)}} \right|$$

$$\simeq \left| \frac{\lambda_j^{(k+1)} - \lambda_j^{(k)}}{\lambda_j^{(k+1)}} \right| \qquad (2.18)$$

The error in $\bar{x}_j^{(k)}$, $\theta_j^{(k)}$, can be approximated by $[\theta_j^{(k)} - \theta_j^{(k+1)}]$ since $\theta_j^{(k+1)} << \theta_j^{(k)}$. Furthermore, from Fig. 1,

$$\theta_j^{(k)} - \theta_j^{(k+1)} \simeq \left[\frac{\sum_{\substack{i=1 \\ i \neq j}}^{n} (\Delta c_{ij}^{(k)})^2}{\sum_{i=1}^{n} (c_{ij}^{(k)})^2} \right]^{1/2}$$

$$= \left[\frac{\Delta \bar{x}_j^{(k)T} B \Delta \bar{x}_j^{(k)}}{\bar{x}_j^{(k)T} B \bar{x}_j^{(k)}} \right]^{1/2} \qquad (2.19)$$

Therefore,

$$\theta_j^{(k)} \simeq \left[\frac{\Delta \bar{x}_j^{(k)T} B \Delta \bar{x}_j^{(k)}}{\bar{x}_j^{(k)T} B \bar{x}_j^{(k)}} \right]^{1/2} \qquad (2.20)$$

The number of operations for the estimation of $\theta_j^{(k)}$ is only about $n\,(2m_b + 3)$, which is small compared with the number of operations per iteration (see Section 2.3).

2.5 Treatment of Missed Eigensolutions

Some of the eigenvalues and corresponding eigenvectors of interest may be missed when the initial approximations are not suitable. In order to check whether this occurs, the Sturm-sequence property [9,31,39,48,51] may be applied. The Sturm-sequence property is expressed as follows: if for an approximate eigenvalue $\lambda_j^{(0)}$, $(A - \lambda_j^{(0)}B)$ is decomposed into LDL^T, where L is a lower triangular matrix and D a diagonal one, then the number of negative elements in D equals the number of eigenvalues smaller than $\lambda_j^{(0)}$. A computed eigenvalue can be checked using the above property with negligible extra computation, since the decomposition of the matrix $(A - \lambda_j^{(0)}B)$ has already been carried out during the procedure for the solution of Eq. (2.7).

If some of the eigenvalues of interest are detected to be missing, finding them consists of three steps: finding approximations to the missed eigenvalues, finding approximate eigenvectors corresponding to the missed eigenvalues, and improving the approximate eigensolutions.

The approximate eigenvalues can be found by the repeated applications of the Sturm-sequence calculation mentioned above and the method of bisection [9,31,38,51], or by the polynomial iteration method [7,8,9,38,51], in which the zeros of the characteristics polynomial $p(\lambda) = \det(A - \lambda B)$ are found using variants of Newton's method.

In the second step, the approximation to the eigenvectors corresponding to the missed eigenvalues is found. Frequently, finding the eigenvectors corresponding to the missed eigenvalues is much more difficult than finding the missed eigenvalues. However, subspace iterations with a shift [6,32], which will be discussed in Chapter 4, or dynamic condensation [34,42,50] may be used for this purpose.

Finally, the approximate eigenvalues and corresponding approximate eigenvectors can be improved by the method of Section 2.2 if the eigenvalues are not multiple or close, or if they are, by the method of Chapter 3.

3. CLOSE OR MULTIPLE ROOTS

3.1 General

As mentioned earlier, the method presented in Chapter 2 fails or exhibits slow convergence if it is applied to the solution for multiple or close eigenvalues and for their corresponding eigenvectors. The failure or slow convergence of the method is caused by impending singularity of the coefficient matrix for the unknown incremental values as the successive approximations approach the true eigenvalue and eigenvector.

The method presented in this chapter overcomes this shortcoming. To accomplish this, all eigenvectors corresponding to multiple or close eigenvalues are found together. As in the method of Chapter 2, this method yields the eigenvalues and corresponding eigenvectors at the same time.

The essence of the method consists first in finding the subspace spanned by the eigenvectors corresponding to multiple or close eigenvalues. The subspace is found using the Newton-Raphson technique in a way suggested by the Robinson-Harris method [44]. If the eigenvalues of interest are multiple, any set of independent vectors spanning subspace are the true eigenvectors, but if the eigenvalues are merely close together, the vectors must be rotated in the subspace to find the true eigenvectors. The eigenvalues are obtained as a by-product of the process of finding the subspace and any subsequent rotation. In this method, any number of close eigenvalues or an eigenvalue of any multiplicity can be found together with the corresponding eigenvectors.

The theoretical background of the method is presented in Section 3.2 The iterative scheme for finding the subspace of the eigenvectors corresponding to multiple or close eigenvalues is given in Section 3.3. The additional treatment required for close eigenvalues and corresponding eigenvectors is the subject of Section 3.4. The convergence rate and the number of operations per iteration are given in Section 3.5.

3.2 Theoretical Background

Let us consider the system treated in Chapter 2, i.e.,

$$A\bar{x}_i = \lambda_i B\bar{x}_i \qquad (i = 1, 2, \ldots, n) \tag{3.1}$$

where A and B are symmetric matrices of order n, and B is positive definite. The $\bar{x}_i$ are eigenvectors, and the λ_i eigenvalues in the order $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.

Let a set S consist of s integers p_j (j = 1, 2, . . . , s), that is, $S = [p_1, p_2, \ldots, p_s]$ where $1 \leq p_j < n$. The s-dimensional subspace spanned by the eigenvectors $\bar{x}_j$ ($j \epsilon S$) where none of the corresponding eigenvalues λ_j ($j \epsilon S$) are close or equal to eigenvalues λ_i ($i \notin S$) is denoted by R. Let us take s vectors y_j ($j \epsilon S$) which are orthonormal with respect to B and are in the neighborhood of the subspace R. This means that if the vector y_j is expanded in a series of true eigenvectors x_i (i = 1, 2,...,n)

$$\bar{y}_j = \sum_{i=1}^{n} c_{ij} \bar{x}_i \qquad (j \epsilon S) \tag{3.2}$$

then, the following relations must be met:

$$\sum_{i \notin S} c_{ij}^2 \ll \sum_{i \in S} c_{ij}^2 \qquad (j \in S) \tag{3.3}$$

Hence, a vector $\bar{y}_j (j \in S)$ needs not be close to one of the $\bar{x}_j (j \in S)$.

With the above definitions, the subspace R of the eigenvectors $\bar{x}_j (j \in S)$ is characterized by the following constrained stationary-value problem: find the stationary values of

$$w = \sum_{j \in S}^{n} \bar{y}_j^T A \bar{y}_j \tag{3.4}$$

subject to

$$\bar{y}_i^T B \bar{y}_j = \delta_{ij} \qquad (i, j \in S) \tag{3.5}$$

where δ_{ij} is the Kronecker delta, i.e., $\delta_{ij} = 1$ for $i = j$, and $\delta_{ij} = 0$ for $i \neq j$. The function w could be regarded as a sum of Rayleigh quotients of the vectors $\bar{y}_j$, since by Eq. (3.5) the denominators of the Rayleigh quotients are equal to unity. The important result that the stationary property characterizes the subspace R is proved as Theorem 1 of Appendix C.

The stationary-value problem may be treated by the method of Lagrange multipliers. Introducing the undetermined multipliers μ_{ij} $(i,j \in S)$ and letting $\mu_{ij} = \mu_{ji}$ (see Eq. (3.5)), we have the Lagrangian

$$L = \sum_{i \in S} \bar{y}_i^T A \bar{y}_i - \sum_{i \in S} \sum_{j \in S} \mu_{ij} (\bar{y}_i^T B \bar{y}_j - \delta_{ij}) \tag{3.6}$$

The problem of Eqs. (3.4) and (3.5) is equivalent to that of solving the unconstrained stationary-value problem for the Lagrangian L. The problem is solved setting the first partial derivatives of L with respect to the unknowns $\bar{y}_j$ and μ_{ij} equal to zero, i.e.,

$$\frac{\partial L}{\partial \bar{y}_j} = 0 \quad ; \quad A\bar{y}_j = \sum_{i \epsilon S} \mu_{ij} B\bar{y}_i \qquad (j \epsilon S) \tag{3.7}$$

$$\frac{\partial L}{\partial \mu_{ij}} = 0 \quad ; \quad \bar{y}_i^T B\bar{y}_j = \delta_{ij} \qquad (i, j \epsilon S) \tag{3.8}$$

Introducing the following notation

$$Y = [\bar{y}_{p_1}, \bar{y}_{p_2}, \ldots, \bar{y}_{p_s}]$$

$$\bar{d}_j^T = (\mu_{p_1 j}, \mu_{p_2 j}, \ldots, \mu_{p_3 j}) \qquad (j = p_1, p_2, \ldots, p_s)$$

$$D = (\bar{d}_{p_1}, \bar{d}_{p_2}, \ldots, \bar{d}_{p_s}) \tag{3.9}$$

we can write Eq. (3.7) in matrix form as

$$A\bar{y}_j = BY\bar{d}_j \qquad (j = p_1, p_2, \ldots, p_s) \tag{3.10}$$

or collectively

$$AY = BYD \tag{3.11}$$

In the same way, Eq. (3.8) can be written as

$$Y^T B Y = I_s \tag{3.12}$$

where I_s is the unit matrix of order s. Hence, the subspace R of the desired eigenvectors can be found by solving Eqs. (3.11) and (3.12). Note that Eqs. (3.11) and (3.12) are nonlinear in D and Y and that there are $s(s+1)/2$ scalar unknown elements in D, since D is symmetric, and $s(s+1)/2$ independent equations in Eq. (3.12). In the next section, the solution of Eqs. (3.11) and (3.12) in the special case that ($j \epsilon S$) are all multiple or close eigenvalues will be discussed.

3.3 The Iterative Scheme

In this section, the application of the Newton-Raphson technique to the solution of Eqs. (3.11) and (3.12) for multiple or close eigenvalues and their corresponding eigenvectors will be presented. To simplify the notation in this discussion, we take the set S = [1,2,...,s], that is, the s lowest eigenvalues are close together, or the multiplicity of the lowest eigenvalue is s. It should be emphasized that this is not restrictive, and the procedure is perfectly applicable to multiple or close eigenvalues in any range.

Assume that the initial values for D and Y, $D^{(0)}$ and $Y^{(0)}$ are available (the solution for the initial values will be discussed in Chapter 4). Furthermore, we assume that the initial vectors in $Y^{(0)}$ are in the neighborhood of the subspace of the eigenvectors $X = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_s]$ and that they

have been orthonormalized with respect to the matrix B, i.e., $Y^{(0)T}BY^{(0)} = I_s$. With the above assumptions, we now apply the Newton-Raphson technique to the solution of Eqs. (3.11) and (3.12). For the general kth iteration step, let

$$\bar{d}_j^{(k+1)} = \bar{d}_j^{(k)} + \Delta\bar{d}_j^{(k)}$$

$$\bar{y}_j^{(k+1)} = \bar{y}_j^{(k)} + \Delta\bar{y}_j^{(k)} \tag{3.13}$$

where $\Delta\bar{d}_j^{(k)}$ and $\Delta\bar{y}_j^{(k)}$ are unknown incremental values for $\bar{d}_j^{(k)}$ and $\bar{y}_j^{(k)}$.

Introducing Eq. (3.13) into Eqs. (3.10) and (3.12) and neglecting the nonlinear terms, we obtain the linear simultaneous equations for $\Delta\bar{d}_j^{(k)}$ and $\Delta\bar{y}_j^{(k)}$:

$$A\Delta\bar{y}_j^{(k)} - BY^{(k)}\Delta\bar{d}_j^{(k)} = -A\bar{y}_j^{(k)} + BY^{(k)}\bar{d}_j^{(k)} + B\Delta Y^{(k)}\bar{d}_j^{(k)} \tag{3.14}$$

$$Y^{(k)T}BY^{(k)} + 2Y^{(k)T}B\Delta Y^{(k)} = I_s \tag{3.15}$$

By Theorem 3 of Appendix C, if the λ_j (j = 1,2,...,s) are multiple or close eigenvalues, the off-diagonal elements of D are zero or very small compared with its diagonal ones, thus the last term of Eq. (3.14) may be approximated by $\mu_{jj}B\,\Delta\bar{y}_j^{(k)}$, yielding

$$(A - \mu_{jj}^{(k)}B)\,\Delta\bar{y}_j^{(k)} - BY^{(k)}\Delta\bar{d}_j^{(k)} = -A\bar{y}_j^{(k)} + BY^{(k)}\bar{d}_j^{(k)} \tag{3.16}$$

Let us take

$$Y^{(k)T}BY^{(k)} = I_s \tag{3.17}$$

Then, Eq. (3.15) becomes

$$Y^{(k)T} B \Delta y_j^{(k)} = 0 \tag{3.18}$$

which is the condition that the incremental vectors be orthogonal to the current vectors with respect to B. If the computational scheme is slightly altered so that the latest $\bar{y}_i^{(k)}$ is used at all times, the orthogonality condition is satisfied automatically provided that the initial vectors $\bar{y}_i^{(0)}$ are orthogonal. What this means is that we use $\bar{y}_i^{(k)}$ $(i = 1,2,\ldots,j-1)$ for the computation of $\bar{y}_j^{(k+1)}$.

The final equations to solve for $\Delta\bar{d}_j^{(k)}$ and $\Delta\bar{y}_j^{(k)}$ are Eqs. (3.16) and (3.18) along with the orthonormality condition, Eq. (3.17). These equations can be written in matrix form as

$$\begin{bmatrix} A - \mu_{jj}^{(k)} B & -BY^{(k)} \\ -Y^{(k)T} B & 0 \end{bmatrix} \begin{bmatrix} \Delta\bar{y}_j^{(k)} \\ \Delta\bar{d}_j^{(k)} \end{bmatrix} = \begin{bmatrix} -\bar{r}_j^{(k)} \\ 0 \end{bmatrix} \tag{3.19}$$

where

$$\bar{r}_j^{(k)} = A\bar{y}_j^{(k)} - BY^{(k)}\,\bar{d}_j^{(k)} \tag{3.20}$$

The coefficient matrix for the unknowns, $\bar{d}_j^{(k)}$ and $\bar{y}_j^{(k)}$, is symmetric. Furthermore, it is nonsingular, as is shown in Appendix A. Thus, Eq. (3.19)

can be solved for $\Delta\bar{d}_j^{(k)}$ and $\Delta\bar{y}_j^{(k)}$, yielding improved values, $\bar{d}_j^{(k+1)}$ and $\bar{y}_j^{(k+1)}$ from Eq. (3.13).

The algorithm using Eq. (3.19) requires a new triangularization in each iteration, since the coefficient matrix is changed in each iteration. It therefore seems useful, as in Chapter 2, to substitute $(A - \mu_{jj}^{(0)}B)$ for $(A - \mu_{jj}^{(k)}B)$ in Eq. (3.19) in order to save computational effort in the solution. That is, the basic equations for the increments are taken as

$$\begin{bmatrix} A - \mu_{jj}^{(0)}B & -BY^{(k)} \\ -Y^{(k)^T}B & 0 \end{bmatrix} \begin{bmatrix} \Delta\bar{y}_j^{(k)} \\ \Delta\bar{d}_j^{(k)} \end{bmatrix} = \begin{bmatrix} -\bar{r}_j^{(k)} \\ 0 \end{bmatrix} \qquad (3.21)$$

where the residual vector $\bar{r}_j^{(k)}$ is defined as in Eq. (3.20). The coefficient matrix in Eq. (3.21) is also symmetric and nonsingular (Appendix A). The equation (3.21) was obtained discarding a small linear term $(\mu_{jj}^{(k)} - \mu_{jj}^{(0)})B\,\bar{y}_j^{(k)}$ of Eq. (3.19). The procedure using Eq. (3.21) requires only partial triangularizations in each iteration, since only the vectors in $Y^{(k)}$ are changed, reducing the number of operations per iteration. The procedure depends, for its convenience, on the decoupling of the $\Delta\bar{y}_j^{(k)}$ for the s vectors $\bar{y}_j^{(k)}$ (i=1,2,...,s). The decoupling was possible only because the small linear terms

$$\sum_{\substack{i=1 \\ i\neq j}}^{n} \mu_{ij}^{(k)}\, B\Delta\bar{y}_j^{(k)}$$

(see Eq. (3.14)) could be dropped for λ_j (j=1, 2, . . . , s) all close together. Experience with Eq. (3.21) for λ_j (j=1, 2, . . . , s) which are not close together indicates that satisfactory results cannot be obtained.

Note that if s = 1, Eqs. (3.19) and (3.21) are equivalent to the equations used for distinct eigenvalues and corresponding eigenvectors: Eq. (3.19) becomes Eq. (2.6), the equations used in the Robinson-Harris method, and Eq. (3.21) becomes Eq. (2.7), used in the proposed method.

With sufficient large k, the incremental values $\Delta\bar{d}_j^{(k)}$ and $\Delta\bar{y}_j^{(k)}$ will vanish. Then, from Eq. (3.21)

$$\lim_{k\to\infty} \bar{r}_j^{(k)} = \lim_{k\to\infty} (A\bar{y}_j^{(k)} - BY^{(k)}\,\bar{d}_j^{(k)}) = 0 \qquad (3.22)$$

Letting

$$\bar{d}_j = \lim_{k\to\infty} \bar{d}_j^{(k)}$$

$$\bar{y}_j = \lim_{k\to\infty} \bar{y}_j^{(k)} \qquad (3.23)$$

we write Eqs. (3.22) and (3.17) as

$$AY = BYD \qquad (3.24)$$

$$Y^TBY = I_s \qquad (3.25)$$

where $Y = (\bar{y}_1,\bar{y}_2,\ldots,\bar{y}_s)$, and $D = (\bar{d}_1,\bar{d}_2,\ldots,\bar{d}_s)$. By Theorem 3 of Appendix C, if the eigenvalues λ_j (j=1,2,...,s) are multiple, the values of the off-diagonal elements of D are all zero, and its diagonal elements have an equal

value which is the desired multiple eigenvalue. Moreover, the vectors in Y are the corresponding eigenvectors. However, if the eigenvalues are close but not equal, additional operations are required to find the desired eigenvalues and eigenvectors. These additional operations are the subject of the next section.

3.4 Treatment of Close Roots

Once the converged solution D and Y has been found by the algorithm described in the previous section, but the values of the off-diagonal elements of D are not zero, the vectors in Y are rotated in the subspace of Y to find the true eigenvectors. A rotation matrix is found by solving a small eigenvalue problem. Furthermore, the eigenvalues of the small eigenvalue problem are the desired eigenvalues. The derivation of the small eigenvalue problem is as follows. The system with the s eigenvectors in $X = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_s]$ and corresponding eigenvalues in $\Lambda = \text{diag}\ (\lambda_1, \lambda_2, \ldots, \lambda_s)$ may be written as

$$AX = BX\Lambda \tag{3.26}$$

where A and B are symmetric matrices of order n. Now, let

$$X = YZ \tag{3.27}$$

where Z is the unknown rotation matrix of order s. Introducing Eq. (3.27) into Eq. (3.26), we get

$$AYZ = BYZ\Lambda \tag{3.28}$$

Postmultiplying Eq. (3.24) by the matrix Z yields

$$AYZ = BYDZ \tag{3.29}$$

Premultiplying Eqs. (3.28) and (3.29) and using $Y^TBY = I_s$ of Eq. (3.25), we obtain the special eigenvalue problem of order s

$$DZ = Z\Lambda \tag{3.30}$$

where D is the converged solution found by the algorithm of the previous section. The matrix D is symmetric (see Eq. (3.24)) and of order s, the number of close eigenvalues, which is usually small. The absolute values of the off-diagonal elements of D are small compared with those of its diagonal elements (see Appendix C). The eigenvalue problem, Eq. (3.30) can be easily solved by any suitable technique such as Jacobi's method [31,51], yielding the desired eigenvalues in Λ $(\lambda_1, \lambda_2, \ldots, \lambda_s)$ and the matrix Z, which in turn gives the eigenvectors X by Eq. (3.27). The number of operations required for the solution of Eq. (3.30) is very small compared with that of Eq. (3.21), since s is small.

3.5 Convergence Rate and Operation Count

In this section, the convergence rates of a multiple eigenvalue and the corresponding eigenvectors found in Appendix B will be summarized. For convenience, we assume that the lowest eigenvalues are multiple, i.e., $\lambda^* = \lambda_1 = \lambda_2 = \ldots = \lambda_s$. Let the approximate eigenvectors $\bar{y}_j^{(k)}$ $(j = 1, 2, \ldots, s)$ be expanded in terms of the eigenvectors $\bar{x}_i$ $(i = 1, 2, \ldots, n)$, i.e.,

$$\bar{y}_j^{(k)} = \sum_{i=1}^{n} c_{ij}^{(k)} \bar{x}_i \qquad j = 1, 2, \ldots, s \tag{3.31}$$

where $c_{ij}^{(k)}$ is a scalar representing the components of the eigenvector $\bar{x}_i$ on $\bar{y}_j^{(k)}$. If $\gamma_j^{(k)}$ denotes the error in $\mu_{jj}^{(k)}$ and $\theta_j^{(k)}$ the error in $\bar{y}_j^{(k)}$, then they may be defined by

$$\gamma_j^{(k)} = \left| \frac{\lambda^* - \mu_{jj}^{(k)}}{\lambda^*} \right| \tag{3.32}$$

$$\theta_j^{(k)} = \left[\sum_{i=s+1}^{n} \left(c_{ij}^{(k)}\right)^2 \right]^{1/2} \Bigg/ \left[\sum_{i=1}^{s} \left(c_{ij}^{(k)}\right)^2 \right]^{1/2} \tag{3.33}$$

As shown in Appendix B, the error in $\mu_{jj}^{(k+1)}$ and $\bar{y}_j^{(k+1)}$ may be written as

$$\gamma_j^{(k+1)} = h^2 \gamma_j^{(k)} \tag{3.34}$$

$$\theta_j^{(k+1)} = h\theta_j^{(k)} \tag{3.35}$$

where

$$h = \max_i \left| \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} \right| << 1 \qquad \begin{array}{l} i = s+1, s+2, \ldots, n; \\ j = 1, 2, \ldots, s \end{array} \tag{3.36}$$

t can be seen from Eqs. (3.34) and (3.35) that the eigenvalues and the corresponding eigenvectors converge linearly. However, the eigenvalues converge much more rapidly than the eigenvectors.

The number of operations N_p required for finding multiple or close eigenvalues and the corresponding eigenvectors is calculated in Table 1. This number is

$$N_p = \frac{1}{2} pn\ (m_a^2 + 3m_a + 2m_b + 2) + T_p n\ [(s+4)\ m_a + 2m_b + \frac{1}{2}\ (s^2 + 7s + 4)] \quad (3.37)$$

where s is the multiplicity of an eigenvalue or the number of close eigenvalues, and T_p is the total number of iterations required for a solution. It can be seen that if s = 1, the number of operations is equal to the number of operations required for finding a simple eigenvalue and the corresponding eigenvector (see Eq. (2.14)).

4. APPROXIMATE STARTING EIGENSOLUTION

4.1 General

The iterative methods described in the previous chapters begin with an approximate starting eigensolution. In this chapter, a procedure to find the starting solution is presented. The approximate starting solution of an eigenvalue problem is often available either as the final answer in some approximate methods or as an intermediate result in other iterative methods.

Numerous methods for approximate solutions have been developed. These include static or dynamic condensation [2,3,25,28,34,42], Rayleigh-Ritz analysis [48,51], component mode analysis [9,51], and related methods summarized by Uhrig [50]. In all these methods, the approximate solution is found in a single step, and not in an iterative process. Hence, automatic improvement of the solution is not built into the procedure. Moreover, the success of the methods depends, to a great extent, on the engineer's judgment, which is difficult to incorporate into an automatic computer program.

Another possible way for finding the approximate solution is to take the intermediate results from other iterative methods such as a method combining the Gram-Schmidt orthogonalization process [51] with simultaneous iteration method or combining Rayleigh-Ritz analysis [6,9,11,29,32,49] with simultaneous iteration method. The latter combined method is sometimes called the "subspace iteration method" [6,9]. The subspace iteration method is used here to find approximate starting solutions because it has a better convergence rate than most others. The method itself turns out to require selecting starting vectors. However, a scheme to find starting vectors for

the subspace iteration method has been well established and is fairly routine (see Section 4.2.2). In the next section, the subspace iteration method will be discussed.

4.2 Subspace Iteration Method

4.2.1 The Iterative Scheme

The subspace iteration method is a repeated application of the classical vector iteration method (power method) and Rayleigh-Ritz analysis. Suppose that the p smallest eigenvalues λ_i (i = 1,2,...,p) and corresponding eigenvectors x_i are required and that we have p initial independent vectors $\bar{x}_i^{(0)}$ (i = 1,2,...,p) spanning a p-dimensional subspace in the neighborhood of the subspace of the desired eigenvectors.

If the approximate eigenvectors and corresponding eigenvalues after k iterations are denoted by $\bar{x}_i^{(k)}$ and $\lambda_i^{(k)}$, $X^{(k)} = [\bar{x}_1^{(k)}, \bar{x}_2^{(k)},\ldots,\bar{x}_p^{(k)}]$, and $D^{(k)} = \text{diag}\,(\lambda_1^{(k)}, \lambda_2^{(k)},\ldots,\lambda_p^{(k)})$, the subspace iteration method for the kth iteration may be described as follows:

(i) Find the improved eigenvectors $Y^{(k)} = [\bar{y}_1^{(k)}, \bar{y}_2^{(k)},\ldots,\bar{y}_p^{(k)}]$ by the simultaneous inverse iteration method;

$$AY^{(k)} = BX^{(k-1)} \tag{4.1}$$

(ii) Compute the projections of the operators A and B onto the subspace spanned by the p vectors in $Y^{(k)}$;

$$\begin{aligned} \overset{*}{A}^{(k)} &= Y^{(k)T} AY^{(k)} \\ \overset{*}{B}^{(k)} &= Y^{(k)T} BY^{(k)} \end{aligned} \tag{4.2}$$

where $\overset{*}{A}^{(k)}$ and $\overset{*}{B}^{(k)}$ are pxp symmetric matrices.

(iii) Solve the eigenvalue problem of reduced order p for the eigenvalues in $D^{(k)} = \text{diag}\ (\lambda_1^{(k)}, \lambda_2^{(k)}, \ldots, \lambda_p^{(k)})$ and the eigenvectors in $Z^{(k)} = [\bar{z}_1^{(k)}, \bar{z}_2^{(k)}, \ldots, \bar{z}_p^{(k)}]$;

$$\overset{*}{A}^{(k)}\ Z^{(k)} = \overset{*}{B}^{(k)}\ Z^{(k)}\ D^{(k)} \tag{4.3}$$

(iv) Find an improved approximation to the eigenvectors;

$$X^{(k)} = Y^{(k)}\ Z^{(k)} \tag{4.4}$$

Then,

$$\lim_{k\to\infty} D^{(k)} = \text{diag}\ (\lambda_1, \lambda_2, \ldots, \lambda_p)$$

$$\lim_{k\to\infty} X^{(k)} = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_p] \tag{4.5}$$

Note that Eqs. (4.2) through (4.4) represent a Rayleigh-Ritz analysis with the vectors in $Y^{(k)}$ as the Ritz basis vectors, which results in $X^{(k)}$, the best approximation to the true eigenvectors in the subspace of $Y^{(k)}$.

More rapid convergence can be obtained by taking more iteration vectors than the number of eigensolutions sought. However, the more starting vectors are taken, the more computational effort is required per iteration. As an optimal number of iteration vectors, q, q = min (2p, p + 8) has been suggested [6,9].

To find eigenvalues within a given range $a < \mu < b$ and the corresponding eigenvectors, we may use, instead of Eq. (4.1), the inverse iteration with a shift [32]:

$$(A - \mu B)\, Y^{(k)} = BX^{(k-1)} \tag{4.6}$$

where μ is a shift and can be taken as $(a + b)/2$. It is clear from Eq. (4.6) that the eigenvectors corresponding to the eigenvalues in the vicinity of a shift μ will converge rapidly. However, the convergence of other eigenvectors may be slower than when the shift is not applied, since as a result of the application of the shift, the absolute values of some shifted eigenvalues may become closer.

4.2.2 Starting Vectors

The number of iterations required for convergence depends on how close the subspace spanned by the starting vectors is to the exact subspace. If approximations to the required eigenvectors are already available, e.g., from a previous solution to a similar problem, these may be used as a set of starting vectors. If not, we may use one of the schemes for generating starting vectors which have been proposed as effective [6,11,32,47].

The scheme for establishing the starting vectors proposed by Bathe and Wilson [6,9] is used here because of its simplicity and effectiveness. The scheme may be described as follows. The first column of $BX^{(0)}$ in Eq. (4.1) is formed simply from the diagonal elements of B. That is, if $BX^{(0)}$ is denoted by C,

$$c_{i1} = b_{ii} \qquad (i = 1,2,\ldots,n) \tag{4.7}$$

This assures that all mass degrees-of-freedom are excited in order not to miss a mode [6,9]. The next (q-1) columns in C may each have all zeros except for a certain coordinate where a one is placed. These coordinates are found in the following way. First, compute the ratios a_{ii}/b_{ii} $(i = 1,2,\ldots,n)$ and take the (q-1) s_j's $(j = 1,2,\ldots,q-1)$ such that the absolute values of the ratios a_{ii}/b_{ii} for i $(i = s_1, s_2,\ldots,s_{q-1})$ are smallest over all i. Then,

$$c_{i,\,j-1} = 1 \quad \text{for} \quad i = s_j \quad (i = 1,2,\ldots,n)$$

$$= 0 \quad \text{for} \quad i \neq s_j \quad (j = 1,2,\ldots,q-1) \qquad (4.8)$$

If the absolute values of the ratios are close or equal, then it was recommended [6,9] that the s_j's $(j = 1,2,\ldots,q-1)$ be chosen so that they are well spaced.

4.2.3 Convergence Rate, Operation Count, and Estimation of Errors

With an adequate choice of the starting vectors, the subspace iteration method gives good approximations to the exact eigenvalues and eigenvectors even after only a few iterations. However, the subsequent convergence is only linear with the rates of convergence equal to λ_i/λ_{q+1} $(i = 1,2,\ldots,p)$ for the ith eigenvector and $(\lambda_i/\lambda_{q+1})^2$ for the corresponding eigenvalue. These ratios indicate that for the higher eigenvalue convergence is slower. Hence, the convergence of the pth mode controls the termination of the iteration process.

One of the most important indicators of the effectiveness of numerical methods is the total number of operations required for finding a solution, which depends on both the rate of convergence and the number of operations per iteration. This number for the subspace iteration method, N_s, (see Table 1) may be expressed by

$$N_s = T_s qn\ (2m_a + 4m_b + 2q + 4) + n\ (m_a^2 + 3m_a + m_b + 1)$$

where m_a and m_b are the half band-widths of A and B, and T_s is the total number of iterations required for the solution.

The total number of iterations T_s, depends on the rate of convergence and tolerances of the errors in approximate eigenvalues and eigenvectors. Bathe and Wilson [6,9] suggested use of the following formula for the estimation of errors in the ith eigenpair at the kth iteration:

$$\left| \frac{\bar{r}_i^{(k)}}{A\bar{x}_i^{(k)}} \right| \tag{4.10}$$

where $\bar{r}_i^{(k)} = (A - \lambda_i^{(k)} B)\ \bar{x}_i^{(k)}$.

The error estimated by Eq. (4.10) is a function of both the approximate eigenvalues and eigenvectors. However, it may be more reasonable to estimate the errors in approximate eigenvalues and eigenvectors using separate formulas as follows: let $\gamma_i^{(k)}$ and $\theta_i^{(k)}$ be the errors in the ith approximate eigenvalue and eigenvector. Then $\gamma_i^{(k)}$ may be estimated by

$$\gamma_i^{(k)} \simeq \frac{\lambda_i^{(k+1)} - \lambda_i^{(k)}}{\lambda_i^{(k+1)}} \qquad (i = 1,2,\ldots,p) \tag{4.11}$$

For the estimate of $\theta_i^{(k)}$, we find the incremental vectors $\Delta x_i^{(k)}$ from the relations

$$\bar{x}_i^{(k+1)} = \alpha_{ii}^{(k)} \bar{x}_i^{(k)} + \Delta \bar{x}_i^{(k)}$$

$$\bar{x}_i^{(k)T} B \, \Delta \bar{x}_i^{(k)} = 0 \tag{4.12}$$

Then,

$$\theta_i^{(k)} \simeq \left| \Delta x_i^{(k)T} B \Delta x_i^{(k)} \right|^{1/2} \Big/ \left| \alpha_{ii}^{(k)2} x_i^{(k)T} B x_i^{(k)} \right|^{1/2} \tag{4.13}$$

If some of the approximate eigenvalues λ_i $(i = p_1, p_2, \ldots, p_s)$ are equal or very close, we may then compute $\Delta \bar{x}_i^{(k)}$ from the relations

$$\bar{x}_i^{(k+1)} = \sum_{j=p_1}^{p_s} \alpha_{ij}^{(k)} \bar{x}_j^{(k)} + \Delta \bar{x}_i^{(k)}$$

$$\bar{x}_j^{(k)T} B \Delta \bar{x}_i^{(k)} = 0 \quad ; \; (j = p_1, p_2, \ldots, p_s)$$

$$\theta_i^{(k)} \simeq \left(\bar{x}_i^{(k)T} B \, \bar{x}_i^{(k)} \right)^{1/2} \Big/ \left(\sum_{j=p_1}^{p_s} \alpha_{ij}^{2(k)} \bar{x}_j^{(k)T} B \bar{x}_j^{(k)} \right)^{1/2} \tag{4.14}$$

For the purpose of comparison of the proposed methods of Chapters 2 and 3 with the subspace iteration method, the errors were computed using Eqs. (4.11) to (4.14).

4.3 Starting Solution for the Proposed Method

The intermediate results from the subspace iteration are used as the starting solutions for the proposed method. During the subspace iterations, the errors in approximate eigenvalues and corresponding eigenvectors can be estimated by the scheme described in Section 4.2.3. Furthermore, these errors can be used for estimating the number of iterations or the number of operations required for the solution by both the subspace iteration method and the proposed method. Hence, it is possible to estimate the optimal number of iterations to be carried out by the subspace iteration method. This optimal number of iterations is usually one or two.

Let λ_i^* and $\bar{x}_i^*$ $(i = 1,2,\ldots,p)$ be the intermediate solutions from the subspace iteration method after the optimal number of iterations. Then, if the λ_i^* are well separated, λ_i^* and $\bar{x}_i^*$ can be taken as the starting solutions for the method of Chapter 2, $\lambda_i^{(0)}$ and $\bar{x}_i^{(0)}$. However, if some of them, e.g., λ_i^* $(i = p_1,p_2,\ldots,p_s)$ are equal or very close, λ_i^* and $\bar{x}_i^*$ are taken as the starting solution for the method of Chapter 3 as

$$y_i^{(0)} = \bar{x}_i^*$$

$$\mu_{ii}^{(0)} = \lambda_i^*$$

$$\mu_{ij}^{(0)} = 0 \quad \text{for } i \neq j \qquad (i,j = p_1,p_2,\ldots,p_s) \quad (4.15)$$

It should be noted that from Eqs. (4.3) and (4.4), the iteration vectors in the subspace iteration method are always orthogonalized with respect to B. Therefore, orthogonalization is not required for the first iteration of the proposed method.

5. NUMERICAL RESULTS AND COMPARISONS

5.1 General

The relative efficiency of the methods developed in this study is illustrated in this chapter by the numerical results of the free vibration analyses of the following example problems:

(a) Ten-Story, Ten-Bay Plane Frame

(b) Two-Hinged Circular Arch

(c) Simply Supported Plate.

The problems were formulated using a stiffness method for the plane frame problem, a finite difference method for the arch problem, and a finite element method for the plate problem. No attempt has been made to present the solutions of eigenvalue problems of very large order, although the proposed method is developed for them. However, some trends can be inferred from the example problems presented here.

The first two problems, with distinct eignevalues, were solved by the method discussed in Chapter 2 and the third one, with multiple or close eigenvalues, by the method of Chapter 3. The above problems were also solved using the Robinson-Harris method [44] and the subspace iteration method discussed in Chapter 4. The results are summarized in Tables 2 through 5. The numerical results given here are shown to be consistent with the convergence estimates of Appendix B.

For each method, the total number of operations required for finding the desired eigenvalues and eigenvectors to the same accuracy was found. These are presented and compared in Table 6. Although a tolerance of 10^{-4} on the eigenvalues and eigenvectors should be sufficient for normal requirements, it

was taken as 10^{-6} for the purpose of comparisons of the convergence characteristics of the methods.

The numerical computations of the above problems were performed on the CDC CYBER 175 system of the Digital Computer Laboratory of the University of Illinois, Urbana, Illinois.

5.2 Plane Frame

The ten-story, ten-bay plane shown in Fig. 2 was taken as an example problem in order to test the method of Chapter 2 for problems with distinct eigenvalues. The problem was formulated by a stiffness method in which the axial deformations of the members are considered, but the shear deformations neglected [40]. The frame with three displacements per joint has a total of 330 degrees of freedom. The mass matrix is the consistent mass matrix [4,5] with a maximum half-bandwidth of 35, equal to that of the stiffness matrix.

The four smallest eigenvalues and their corresponding eigenvectors were computed by the proposed method, by the Robinson-Harris method, and by the subspace iteration method. The results are given in Table 2. For the subspace iteration method, ten starting vectors were formed by the technique suggested by Bathe and Wilson (see Section 4.2.2). The starting approximate eigenvalues and eigenvectors for the proposed method and for the Robinson-Harris method were established by performing two cycles of subspace iteration. Table 2 shows that even the eigenvalues calculated by two subspace iterations are already accurate to three figures. However, the eigenvectors are accurate to only one or two figures. In addition, the convergence of eigenvectors by the subspace iteration method is so slow, as discussed in Section 4.2.3, that 12 iterations were required for the convergence of both eigenvalues and eigen-

vectors to the indicated tolerance. The proposed method and the Robinson-Harris method required only two iterations for the convergence of eigenpairs except for that of the fourth mode, which required four iterations by the proposed method and three iterations by the Robinson-Harris method.

The total number of operations to solve for all the desired eigenpairs by the proposed method is 3.50×10^6; by the Robinson-Harris method, 4.57×10^6, and by the subspace iteration method, 9.27×10^6. Therefore, the Robinson-Harris method required 1.31 times as many operations as the proposed method did, and the subspace iteration method required 2.78 times as many operations, as shown in Table 6.

5.3 Arch

A uniform 90 degree circular arch simply supported at both ends was analyzed for in-plane vibration behavior. The arch has the radius a and the thickness h, and the ratio a/h = 20. Melin and Robinson [36] investigated the free vibration behavior of such an arch as a part of a study of vibrations of a simply supported cylindrical shell using a finite difference method. The arch was divided into 12 uniform segments giving 22 degrees of freedom. The maximum half-bandwidth of the stiffness matrix is four and the mass matrix is a unit diagonal matrix.

The problem was analyzed for the three smallest eigenvalues and their eigenvectors by the proposed method, by the Robinson-Harris method, and by the subspace iteration method. The results are summarized in Table 3. Five radial displacements were taken as master displacements for the iteration vectors of the subspace iteration method. Starting approximate eigenpairs for the proposed method and the Robinson-Harris method were established by carrying out just one cycle of the subspace iteration.

The comparison of the total number of operations for each method is given in Table 6. The proposed method needed 8.87×10^3 operations, the Robinson-Harris method $9.77 \times .0^3$ operations, and the subspace iteration method 1.76×10^4 operations. Hence, the ratio of the total number of operations by the Robinson-Harris method to that by the proposed method is 1.10, and this ratio for the subspace iteration method is 1.98.

5.4 Plate Bending

A plate simply supported on all edges was analyzed in order to test the method presented in Chapter 3, for the solution of eigenvalue problems with multiple or close eigenvalues. The plate has the lengths a and b, and the theckness h. Two special cases were considered; an aspect ratio b/a of 1.00 and b/a equal to 1.01. The first case gives multiple roots, while the second one gives close roots. The problem was formulated by a finite element method, in which the plate was divided into 16 elements. Each unrestarined node has a deflection and two rotational displacements, giving a total of 39 degrees of freedom. The mass matrix is the consistent mass matrix [4,5] with a maximum half-bandwidth of 16, equal to that of the stiffness matrix.

The four smallest eigenvalues and corresponding eigenvectors were computed for both cases by the proposed method and by the subspace iteration method. The results are summarized in Tables 4 and 5. the deflection at each node was taken as the master degrees of freedom, giving nine iteration vectors for the subspace iteration method. Only one cycle of subspace iteration was performed for the proposed method. The multiple eigenvalues of the square plate and the close eigenvalues of the rectangular plate were isolated by the method discussed in Chapter 3.

The total number of operations by the proposed method for both cases is 1.27×10^5 and by the subspace iteration method, 2.20×10^5, as shown in Table 6. Hence, the subspace iteration method needed 1.73 times as many operations as the proposed method did.

5.5 Comparison between the Theoretical Convergence Rates and Numerical Results

It was shown in the previous chapters that in the proposed method, the convergence of eigenvalues is much faster than that of eigenvectors. Hence, the convergence of the eigenvectors governs the termination of process, when the tolerances on the eigenvalues and eigenvectors are same. Comparison between the theoretical convergence rates and numerical results was, therefore, carried out only for the eigenvectors. Comparisons between the proposed method and subspace iteration method are given in Tables 7, 8, and 9.

The numerical convergence rates were computed by $\theta_i^{(k+1)}/\theta_i^{(k)}$, where $\theta_i^{(k)}$ is the error on the ith approximate eigenvector at the kth iteration. These errors are given in Tables 2 through 5, showing that the numerical convergence rates for the proposed method and the subspace iteration method increase monotonically to approach the theoretical convergence rates as the number of iterations increases. A typical example for this is the convergence rates of the fourth eigenvector of the frame problem, as shown in Table 7. The number of iterations for this mode is large enough to provide a good comparison between the theoretical and numerical convergence rates.

Tables 7, 8, and 9 show that in the proposed method, eigenpairs converge much faster than in the subspace iteration method. Note also that in Table 9, the numerical convergence rates for the proposed method are almost same as

those rates for the problem with double roots. Hence, the expressions for the theoretical convergence rates for multiple eigenvalues also seem applicable to the case of close eigenvalues.

6. SUMMARY AND CONCLUSIONS

6.1 Summary of the Proposed Method

Two iterative procedures for the solution of linear eigenvalue problems for systems with a finite number of degrees of freedom were discussed in Chapters 2 and 3. Chapter 2 developed a procedure for finding distinct eigenvalues and the corresponding eigenvectors, and Chapter 3 dealt with multiple or close eigenvalues and the corresponding eigenvectors.

For distinct eigenvalues and the corresponding eigenvectors, the Robinson-Harris method [44] was modified to save overall computational effort by the use of a "modified" form of the Newton-Raphson technique. The modified method reduces both the number of operations per iteration and the convergence rates. However, the reduction of the number of operations generally compensates for the disadvantage of the decrease of the convergence rate, reducing the total number of operations.

The procedure in Chapter 2 for finding a distinct eigenvalue and the corresponding eigenvector fails if the eigenvalue is one of multiple or close eigenvalues, because the matrix involved in the computation become ill-conditioned. This difficulty has been overcome by the new method of Chapter 3. In this mehtod, all eigenvalues close to an eigenvalue or a multiple eigenvalue and the corresponding eigenvectors are found in a group. In other words, a subspace spanned by the approximate eigenvectors is projected by iterations onto the subspace of the exact eigenvectors. If the eigenvalues are multiple, the vectors spanning the subspace are exact eigenvectors. However, if the eigenvalues are close, the exact eigenvectors are found by a simple rotation of the vectors in the subspace. The rotation matrix is found from a special

eigenvalue problem of small order s, the number of the close eigenvalues. The eigenvalues of the small eigenvalue problem are exact eigenvalues of the original system.

The above procedures of the successive approximations require initial approximations to the eigenvalues and eigenvectors. These are available either as the final solution in some approximate methods such as static or dynamic condensation or as an intermediate result in an iterative method as the subspace iteration method described in Chapter 4.

6.2 Conclusions

The method presented in this study is very efficient for finding a limited number of soltutions of eigenvalue problems of large order arising from the linear dynamic analysis of structures. The features of the method are summarized as follows.

(a) The method has very high convergence rates for eigenvalues and eigenvectors. The method is more economical than the subspace iteration method, the advantage being greater in larger problems. For comparable accuracy, a ten-story ten-bay frame required only 36% of the number of operations need in applying subspace iterations.

(b) A transformation to the special eigenvalue problem is not required. Thus, the characteristics of the given matrices such as the sparseness, bandness, and symmetry are preserved, minimizing the storage requirements and the number of operations.

(c) Any number of multiple or close eigenvalues and their eigenvectors can be found. The existence of the multiple or close eigenvalues can be detected during the iterations by the method of Chapter 2.

(d) The eigenvalues in any range of interest and their eigenvectors can be found, if approximations to the solution are known.

(e) The solution can be checked to determine if some eigenvalues and corresponding eigenvectors of interest have been missed, without extra operations.

6.3 Recommendations for Further Study

Several possible areas of further study to improve the proposed method may be suggested.

(a) The convergence rate may be improved by other modifications of the successive approximation method used for the proposed method.

(b) Further improvements may be possible for the method of finding an initial approximation to the eigensolution, and for isolating the eigenvalues and their eigenvectors which may be missed by the proposed method.

(c) The proposed method may be applied to other practical problems of our interest such as a stability analysis of structures.

(d) The proposed method could be easily extended to the continuous eigenvalue problems if there were better ways of direct estimation of their eigensolutions.

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APPENDIX A

NONSINGULARITY OF THE COEFFICIENT MATRICES OF THE BASIC EQUATIONS

Consider the basic equations (3.19) used for finding multiple or close eigenvalues and corresponding eigenvectors of the system

$$A\bar{x} = \lambda B\bar{x} \tag{A.1}$$

in which A and B are symmetric and both of order n, and B is positive definite.

Let the coefficient matrix of Eq. (3.19) be denoted by F, that is

$$F = \begin{bmatrix} A - \mu_{ii}^{(0)} B & \vdots & -BY^{(k)} \\ \cdots & \vdots & \cdots \\ -Y^{(k)^T} B & \vdots & 0 \end{bmatrix} \quad i = m, m+1, \ldots, m+s-1 < n \tag{A.2}$$

where $\mu_{ii}^{(0)}$ $(i = m, m+1, \ldots, m+s-1)$ are initial approximate values of the multiple or close eigenvalues λ_i $(i = m, m+1, \ldots, m+s-1)$, and the s vectors in $Y^{(k)} = [\bar{y}_m^{(k)}, \bar{y}_{m+1}^{(k)}, \ldots, \bar{y}_{m+s-1}^{(k)}]$ are approximate values of the eigenvectors in $X = [\bar{x}_m, \bar{x}_{m+1}, \ldots, \bar{x}_{m+s-1}]$. Note that F is an $(n+s)x(n+s)$ symmetric matrix.

The determinant of F is a continuous function of the approximate eigenvalue and eigenvectors. Hence, if F is nonsingular when the approximate

values in F become the exact ones, then it will be also nonsingular for close enough approximations. It is therefore sufficient for our purpose to use the exact eigenvalue and eigenvectors in Eq. (A.2) to prove nonsingularity. Let us take m = 1 for the convenience of the following presentation, then the resulting matrix G will be

$$G = \begin{bmatrix} A - \lambda_i B & - BX \\ \hline - X^T B & 0 \end{bmatrix} \quad (i = 1,2,\ldots,s) \tag{A.3}$$

where $X = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_s]$.

To find the determinant of G, we follow the idea that Robinson and Harris [44] used for showing the nonsingularity of the coefficient matrix of Eq. (2.10), that is, we consider the eigenvalues γ's and corresponding eigenvectors $\bar{u}$'s of the system

$$G\bar{u} = \gamma \overset{*}{B}\bar{u} \tag{A.4}$$

or collectively

$$GU = \overset{*}{B}UD \tag{A.5}$$

where

$$B^* = \begin{bmatrix} B & 0 \\ \hline 0 & I_s \end{bmatrix}$$

$$U = (\bar{u}_1, \bar{u}_2, \ldots, \bar{u}_s$$

$$D = \text{diag}\ (\lambda_1, \lambda_2, \ldots, \lambda_s)$$

$$I_s = \text{unit matrix of order } s$$

It may be verified by direct substitution that the $(n+s)$ eigenvectors $\bar{u}$'s and their corresponding eigenvalues γ's of Eq. (A.4) are:

$$\bar{u}: \quad \begin{bmatrix} \bar{x}_j \\ \\ \bar{e}_j \end{bmatrix} \qquad \begin{bmatrix} \bar{x}_j \\ \\ -e_j^* \end{bmatrix} \qquad \begin{bmatrix} \bar{x}_k \\ \\ 0 \end{bmatrix} \qquad \begin{matrix} j = 1,2,\ldots,s \\ k = s+1, s+2, \ldots, n \end{matrix}$$

$$\gamma: \quad \left(-\frac{1}{e_{jj}}\right)\left(e_{jj}\right)\left(\lambda_k - \lambda_i\right) \tag{A.6}$$

where λ_i and $\bar{x}_i$ are the eigenvalues and eigenvectors of the system $A\bar{x} = \lambda B\bar{x}$. The vectors $\bar{e}_j$ and $\bar{e}_j^*$ form the diagonal matrices E and E^* such that

$$E = [\bar{e}_1, \bar{e}_2, \ldots, \bar{e}_s] = \text{diag}\ (e_{11}, e_{22}, \ldots, e_{ss})$$

$$E^* = [\bar{e}_1^*, \bar{e}_2^*, \ldots, \bar{e}_s^*] = \text{diag}\ \left(\frac{-1}{e_{11}}, \frac{-1}{e_{22}}, \ldots, \frac{-1}{e_{ss}}\right)$$

$$e_{jj} = \frac{\Delta_{ji} + \sqrt{\Delta_{ji}^2 + 4}}{2} \qquad j = 1,2,\ldots,s$$

$$\Delta_{ji} = \lambda_j - \lambda_i \qquad i,j = 1,2,\ldots,s \tag{A.7}$$

From Eqs. (A.5), (A.6), and (A.7)

$$\det G = (\det B^{*})\,(\det D)$$

$$= (-1)^{s}\,(\det B) \prod_{k=s+1}^{n} (\lambda_k - \lambda_i) \qquad (A.8)$$

In a similar way, the determinant of G for general $m > 1$ is

$$\det G = (-1)^{s}\,(\det B) \prod_{\substack{k=1 \\ k \notin S}}^{n} (\lambda_k - \lambda_i) \qquad (A.9)$$

where the set $S = [m, m+1, \ldots, m+s-1]$. The matrix B is positive definite, which implies that $\det B > 0$. Thus, if λ_i $(i \in S)$ is not equal or close to any of λ_k $(k = 1,2,\ldots,n;\ k \notin S)$, the determinant of G is never equal to zero or close to zero, independently of whether λ_i $(i \in S)$ are close, multiple, or distinct.

From Eq. (A.2), if $s = 1$, the matrix F becomes the coefficient matrix of Eq. (2.10), and by Eq. (A.9), the determinant of the matrix can be approximated by

$$F = (-1)\,(\det B) \prod_{\substack{k=1 \\ k \neq m}}^{n} (\lambda_k - \lambda_m) \qquad (A.10)$$

Therefore, if $\lambda_m \neq \lambda_{m-1}$ and $\lambda_m \neq \lambda_{m+1}$, the matrix F is also nonsingular.

APPENDIX B

CONVERGENCE ANALYSIS

The convergence analysis of the methods introduced in Chapters 2 and 3 will be presented. The eigenvalue problem we deal with here is

$$A\bar{x}_i = \lambda_i B\bar{x}_i \quad (i = 1,2,\ldots,n) \tag{B.1}$$

in which A and B are symmetric matrices of order n, and B is positive definite. The eigenvectors $\bar{x}_i$ $(i = 1,2,\ldots,n)$ are assumed to be orthonormalized with respect to B.

B.1 Case of a Distinct Root

Let us rewrite Eq. (2.7) used for improving approximate values of a distinct eigenvalue λ_j and the corresponding eigenvector $\bar{x}_j$ of the system represented by Eq. (B.1):

$$(A - \lambda_j^{(0)}B)\,\Delta\bar{x}_j^{(k)} - \Delta\lambda_j^{(k)}\,B\bar{x}_j^{(k)} = -(A - \lambda_j^{(k)}B)\,\bar{x}_j^{(k)} \tag{B.2}$$

$$\bar{x}_j^{(k)T} B\Delta\bar{x}_j^{(k)} = 0 \tag{B.3}$$

where $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$ are approximate values of λ_j and $\bar{x}_j$ after k iterations, and $\Delta\lambda_j^{(k)}$ and $\Delta\bar{x}_j^{(k)}$ are unknown incremental values of $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$.

Let the approximate eigenvector $\bar{x}_j^{(k)}$ and the incremental vector $\Delta\bar{x}_j^{(k)}$ be expanded in a series of the true eigenvectors, i.e.,

$$\bar{x}_j^{(k)} = \sum_{i=1}^{n} c_{ij}^{(k)} \bar{x}_i$$

$$\Delta\bar{x}_j^{(k)} = \sum_{i=1}^{n} \Delta c_{ij}^{(k)} \bar{x}_i \tag{B.4}$$

in which $c_{ij}^{(k)}$ and $\Delta c_{ij}^{(k)}$ are scalar coefficients. Since the $\tilde{x}_j^{(k)}$ is in the vicinity of $\bar{x}_j$,

$$\max_{\substack{i \\ i \neq j}} \left| \frac{c_{ij}^{(k)}}{c_{jj}^{(k)}} \right| = \varepsilon << 1 \tag{B.5}$$

The errors in $\lambda_j^{(k)}$ and $\bar{x}_j^{(k)}$, $\gamma_j^{(k)}$ and $\theta_j^{(k)}$, may be defined by

$$\gamma_j^{(k)} = \left| \frac{\lambda_j - \lambda_j^{(k)}}{\lambda_j} \right| << 1$$

$$\theta_j^{(k)} = \left\{ \sum_{\substack{i=1 \\ i \neq j}}^{n} c_{ij}^2(k) \Big/ c_{jj}^2(k) \right\}^{1/2} << 1 \tag{B.6}$$

where the values of $\gamma_j^{(k)}$ and $\theta_j^{(k)}$ are very small compared with unity. If the vectors $\bar{c}_j^{(k)}$ and $\bar{c}_j^{*(k)}$ are defined by

$$\bar{c}_j^{(k)T} = (c_{1j}^{(k)}, c_{2j}^{(k)}, \ldots, c_{nj}^{(k)})$$

$$\bar{c}_j^{*(k)T} = (0, 0, c_{jj}^{(k)}, 0, \ldots, 0) \qquad (B.7)$$

The $\theta_j^{(k)}$ then represents very closely the angle between the vectors $\bar{c}_j^{(k)}$ and $\bar{c}_j^{*(k)}$ (see Fig. 1). The task here is to estimate $\gamma_j^{(k+1)}$ and $\theta_i^{(k+1)}$, the errors in $\lambda_j^{(k-1)}$ and $\bar{x}_j^{(k-1)}$.

Let us substitute Eq. (B.4) into Eqs. (B.2) and premultiply by $\bar{x}_i^T$ to obtain

$$(\lambda_j - \lambda_j^{(0)})\, \Delta c_{ij}^{(k)} - \Delta\lambda_j^{(k)} c_{ij}^{(k)} = -(\lambda_i - \lambda_j^{(k)})\, c_{ij}^{(k)}$$

$$(i = 1, 2, \ldots, n) \qquad (B.8)$$

Substitution of Eq. (B.4) into Eq. (B.3) and use of the orthonormality of the eigenvectors with respect to B results in

$$\sum_{i=1}^{n} c_{ij}^{(k)}\, \Delta c_{ij}^{(k)} = 0 \qquad (B.9)$$

The unknown quantities, $\Delta\lambda_j^{(k)}$ and $\Delta c_{ij}^{(k)}$ will be found from Eqs. (B.8) and (B.9).

From Eq. (B.8)

$$\Delta c_{ij}^{(k)} = \frac{\Delta\lambda_j^{(k)} - (\lambda_i - \lambda_j^{(k)})}{\lambda_i - \lambda_j^{(0)}} c_{ij}^{(k)} \qquad (i = 1, 2, \ldots, n) \qquad (B.10)$$

Now introduce Eq. (B.10) into Eq. (B.9) to obtain

$$(1 + \alpha)\, \Delta\lambda_j^{(k)} = \lambda_j - \lambda_j^{(k)} + (\lambda_j - \lambda_j^{(0)})\beta \qquad (B.11)$$

where

$$\alpha = \sum_{\substack{i=1 \\ i \neq j}}^{n} \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_i - \lambda_j^{(0)}} \left\{ \frac{c_{ij}^{(k)}}{c_{jj}^{(k)}} \right\}^2$$

$$\beta = \sum_{\substack{i=1 \\ i \neq j}}^{n} \frac{\lambda_i - \lambda_j^{(k)}}{\lambda_i - \lambda_j^{(0)}} \left\{ \frac{c_{ij}^{(k)}}{c_{jj}^{(k)}} \right\}^2 \qquad (B.12)$$

Using Eqs. (B.5) and (B.6), we get

$$| \alpha | \leq h\, \theta_j^{2(k)} \ll 1$$

$$| \beta | \leq g\, \theta_j^{2(k)} \ll 1 \qquad (B.13)$$

where

$$h = \max_{\substack{i \\ i \neq j}} \left| \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_i - \lambda_j^{(0)}} \right| << 1$$

$$g = \max_{\substack{i \\ i \neq j}} \left| \frac{\lambda_j - \lambda_j^{(k)}}{\lambda_i - \lambda_j^{(0)}} \right| \simeq 1 \qquad (i = 1, 2, \ldots, n) \qquad (B.14)$$

Therefore, from Eq. (B.11), the $\Delta\lambda_j^{(k)}$ may be approximated by

$$\Delta\lambda_j^{(k)} = \lambda_j - \lambda_j^{(k)} + (\lambda_j - \lambda_j^{(0)})\beta \qquad (B.15)$$

or

$$\lambda_j^{(k+1)} = \lambda_j^{(k)} + \Delta\lambda_j^{(k)}$$

$$= \lambda_j + (\lambda_j - \lambda_j^{(0)})\beta \qquad (B.16)$$

Substitute Eq. (B.15) into Eq. (B.10) to obtain

$$\Delta c_{ij}^{(k)} = - c_{ij}^{(k)} + \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_i - \lambda_j^{(0)}} (1 + \beta) c_{ij}^{(k)}$$

$$(i = 1, 2, \ldots, n) \qquad (B.17)$$

or

$$c_{ij}^{(k+1)} = c_{ij}^{(k)} + \Delta c_{ij}^{(k)}$$

$$= \frac{\lambda_i - \lambda_j^{(0)}}{\lambda_i - \lambda_j^{(0)}} (1 + \beta)\, c_{ij}^{(k)} \qquad (i = 1, 2, \ldots, n) \qquad (B.18)$$

from which, it follows that

$$c_{jj}^{(k+1)} = (1 + \beta)\, c_{ij}^{(k)} \qquad (B.19)$$

The measure of the error in $\bar{x}_j^{(k+1)}$, $\theta_j^{(k+1)}$, can now be found:

$$\theta_j^{(k+1)} = \sum_{\substack{i=1 \\ i \neq j}}^{n} \left\{ \left(\frac{c_{ij}^{(k+1)}}{c_{jj}^{(k+1)}} \right)^2 \right\}^{1/2}$$

$$= \sum_{\substack{i=1 \\ i \neq j}}^{n} \left\{ \left(\frac{\lambda_j - \lambda_j^{(0)}}{\lambda_i - \lambda_j^{(0)}} \right)^2 \left(\frac{c_{ij}^{(k)}}{c_{jj}^{(k)}} \right)^2 \right\}^{1/2}$$

$$\leq h\, \theta_i^{(k)} \qquad (B.20)$$

where h is given in Eq. (B.14) and is very small compared with unity. To find $\gamma_j^{(k+1)}$, the measure of the error of $\lambda_j^{(k+1)}$, we use Eqs. (B.6) and (B.16), giving

$$\gamma_j^{(k+1)} = \left| \frac{\lambda_j - \lambda_j^{(k+1)}}{\lambda_j} \right|$$

$$= \left| \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_j} \beta \right|$$

$$\leq \left| \frac{\lambda_j \quad \lambda_j^{(0)}}{\lambda_j} \right| g \, \theta_j^{2(k)} \qquad \text{(B.21)}$$

by which

$$\gamma_j^{(k+2)} \leq \left| \frac{\lambda_j - \lambda_j^{(0)}}{\lambda_j} \right| g \, \theta_j^{2(k+1)} \qquad \text{(B.22)}$$

Substitution of Eq. (B.20) into Eq. (B.22) and use of Eq. (B.21) results in

$$\gamma_j^{(k+2)} = h^2 \, \gamma_j^{(k+1)} \qquad \text{(B.23)}$$

Hence, it can be seen from Eqs. (B.20) and (B.23) that the j^{th} eigenvector and eigenvalue converge linearly with errors multiplied by h $(h << 1)$ and h^2 respectively in each iteration.

B.2 Case of a Multiple Root

The convergence analysis of the method for finding a multiple eigenvalue and the corresponding eigenvectors of the system given in Eq. (B.1) will now be presented.

For convenience, but without loss of generality, the s lowest eigenvalues are assumed to be equal, and the eigenvalue of multiplicity s is denoted by λ^*, i.e., $\lambda^* = \lambda_1 = \lambda_2 = \ldots = \lambda_s$. Let us rewrite Eqs. (3.21) and (3.17), which are the basic equations for improving approximate values of the multiple eigenvalue and corresponding eigenvectors, i.e.,

$$(A - \mu_{jj}^{(0)} B)\, \Delta\bar{y}_j^{(k)} - BY^{(k)}\, \Delta\bar{d}_j^{(k)} = BY^{(k)}\, \bar{d}_j^{(k)} - A\, \bar{y}_j^{(k)}$$

$$(j = 1, 2, \ldots, s) \qquad \text{(B.24)}$$

$$Y^{(k)T} B\, \Delta\bar{y}_j^{(k)} = 0 \qquad (j = 1, 2, \ldots, s) \qquad \text{(B.25)}$$

and

$$Y^{(k)T} BY^{(k)} = I_s \qquad \text{(B.26)}$$

where I_s is the unit matrix of order s, and

$$Y^{(k)} = [\bar{y}_1^{(k)}, \bar{y}_2^{(k)}, \ldots, \bar{y}_s^{(k)}]$$

$$\bar{d}_j^{(k)T} = (\mu_{1j}^{(k)}, \mu_{2j}^{(k)}, \ldots, \mu_{sj}^{(k)})$$

$$\Delta\bar{d}_j^{(k)T} = (\Delta\mu_{1j}^{(k)}, \Delta\mu_{2j}^{(k)}, \ldots, \Delta\mu_{sj}^{(k)}) \qquad \text{(B.27)}$$

The $\mu_{jj}^{(k)}$ $(j = 1, 2, \ldots, s)$ are approximations to the multiple eigenvalue $\lambda^* = \lambda_1 = \lambda_2 = \ldots = \lambda_s$, and the $\bar{y}_j^{(k)}$ $(j = 1, 2, \ldots, s)$ are approximations

to the true eigenvectors $\bar{x}_j$ (j = 1, 2,...,s). The $\Delta\bar{y}_j^{(k)}$ and $\Delta\bar{d}_j^{(k)}$ are unknown incremental vectors for $\bar{y}_j^{(k)}$ and $\bar{d}_j^{(k)}$.

Let the approximate eigenvectors $\bar{y}_j^{(k)}$ and the incremental vectors $\Delta\bar{y}_j^{(k)}$ be expanded in a series of the true eigenvectors $\bar{x}_i$ (i = 1, 2,...,n), as in Eq. (B.4), i.e.,

$$\bar{y}_j^{(k)} = \sum_{i=1}^{n} c_{ij}^{(k)} \bar{x}_i$$

$$\Delta\bar{y}_j^{(k)} = \sum_{i=1}^{n} \Delta c_{ij}^{(k)} \bar{x}_i \qquad (j = 1, 2,...,s) \qquad \text{(B.28)}$$

Denoting the errors in $\mu_{jj}^{(k)}$ and $\bar{y}_j^{(k)}$ by $\gamma_j^{(k)}$ and $\theta_j^{(k)}$, we have

$$\gamma_j^{(k)} = \left| \frac{\lambda_j - \mu_{jj}^{(k)}}{\lambda_j} \right|$$

$$\theta_j^{(k)} = \frac{\beta_j^{(k)}}{\alpha_j^{(k)}} << 1 \qquad \text{(B.29)}$$

where

$$\alpha_j^{(k)} = \left\{ \sum_{i=1}^{s} c_{ij}^2 (k) \right\}^{1/2}$$

$$\beta_j^{(k)} = \left\{ \sum_{i=s+1}^{n} c_{ij}^2 (k) \right\}^{1/2} \qquad \text{(B.30)}$$

The task here is to estimate the values of $\gamma_j^{(k+1)}$ and $\theta_j^{(k+1)}$. Now let the vectors $\bar{c}_j^{(k)}$ and $\Delta\bar{c}_j^{(k)}$, and the matrix $C^{(k)}$ be

$$\bar{c}_j^{(k)T} = (c_{1j}^{(k)}, c_{2j}^{(k)}, \ldots, c_{nj}^{(k)})$$

$$\Delta\bar{c}_j^{(k)T} = (\Delta c_{1j}^{(k)}, \Delta c_{2j}^{(k)}, \ldots, \Delta c_{nj}^{(k)})$$

$$C^{(k)} = [\bar{c}_1^{(k)}, \bar{c}_2^{(k)}, \ldots, \bar{c}_s^{(k)}] \qquad \text{(B.31)}$$

Then, defining the matrix $X = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n]$, we may write Eq. (B.28) as

$$\bar{y}_j^{(k)} = X\,\bar{c}_j^{(k)} \qquad (j = 1, 2, \ldots, s) \qquad \text{(B.32)}$$

or

$$\gamma^{(k)} = X\,C^{(k)} \qquad \text{(B.33)}$$

and

$$\Delta\bar{y}_j^{(k)} = X\,\Delta\bar{c}_j^{(k)} \qquad (j = 1, 2, \ldots, s) \qquad \text{(B.34)}$$

Substitution of Eqs. (B.32) - (B.34) into Eqs. (B.24) - (B.26), and pre-multiplication of Eq. (B.24) by X^T results in

$$(\Lambda - \mu_{jj}^{(0)}\, I_n)\,\Delta\bar{c}_j^{(k)} - C^{(k)}\,\Delta\bar{d}_j^{(k)} = C^{(k)}\,\bar{d}_j^{(k)} - \Lambda\,\bar{c}_j^{(k)} \qquad \text{(B.35)}$$

$$C^{(k)T}\,\Delta\bar{c}_j^{(k)} = 0 \qquad \text{(B.36)}$$

$$C^{(k)T}\,C^{(k)} = I_s \qquad \text{(B.37)}$$

where

$$\Lambda = \text{diag}\ (\lambda_1, \lambda_2, \ldots, \lambda_n)$$

$$I_n = \text{unit matrix of order n.}$$

Let us find $\Delta\bar{c}_j^{(k)}$ and $\Delta\bar{d}_j^{(k)}$ using Eqs. (B.35) - (B.37). From Eq. (B.35)

$$\Delta\bar{c}_j^{(k)} = (\Lambda - \mu_{jj}^{(0)}\ I_n)^{-1}\ (C^{(k)}\ \bar{d}_j^{(k+1)} - \Lambda\ \bar{c}_j^{(k)}) \qquad (B.38)$$

Substitution of Eq. (B.38) into Eq. (B.36) leads to

$$F^{(k)}\ \bar{d}_j^{(k+1)} = \bar{g}_j^{(k)} \qquad (B.39)$$

where

$$F^{(k)} = C^{(k)^T}\ (\Lambda - \mu_{jj}^{(0)}\ I_n)^{-1}\ C^{(k)}$$

$$\bar{g}_j^{(k)} = C^{(k)^T}\ (\Lambda - \mu_{jj}^{(0)}\ I_n)^{-1}\Lambda\ \bar{c}_j^{(k)} \qquad (B.40)$$

Note that $F^{(k)}$ is a symmetric matrix of order s. Using Eq. (B.33), we can show that

$$F^{(k)} = \frac{1}{\lambda^* - \mu_{jj}^{(0)}}\ R^{(k)}\ (I_s + E^{(k)})\ R^{(k)} \qquad (B.41)$$

where

$$R^{(k)} = \text{diag}\ (\alpha_1^{(k)}, \alpha_2^{(k)}, \ldots, \alpha_s^{(k)}) \qquad (B.42)$$

and the $(\ell, m)^{th}$ element of the symmetric matrix $E^{(k)}$, $e_{\ell m}^{(k)}$, is

$$e_{mm}^{(k)} = \sum_{i=s+1}^{n} \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} \left(\frac{c_{im}^{(k)}}{\alpha_m^{(k)}}\right) \qquad (m = 1, 2,\ldots,s)$$

$$e_{\ell m}^{(k)} = \sum_{i=s+1}^{n} \frac{\lambda^* - \lambda_i}{\lambda_i - \mu_{jj}^{(0)}} \left(\frac{c_{i\ell}^{(k)}}{\alpha\ell^{(k)}}\right) \left(\frac{c_{im}^{(k)}}{\alpha_m^{(k)}}\right)$$

$$(\ell, m = 1, 2,\ldots,s;\ \ell \neq m) \quad \text{(B.43)}$$

The $\alpha_i^{(k)}$ $(i = 1, 2,\ldots,s)$ of Eq. (B.42) are defined in Eq. (B.30). By Eq. (B.29), the absolute values of $e_{\ell m}^{(k)}$ $(\ell, m = 1, 2,\ldots,s)$ are very small compared with unity, thus

$$F^{(k)} \simeq \left(\frac{1}{\lambda^* - \mu_{jj}^{(0)}}\right) \text{diag}\,(\alpha_1^{2(k)}, \alpha_2^{2(k)},\ldots,\alpha_s^{2(k)}) \qquad \text{(B.44)}$$

Similarly, the values of the s components of the vector $\bar{g}_j^{(k)}$ can be found from Eq. (B.40), i.e.,

$$g_{jj}^{(k)} = \frac{\alpha_j^{2(k)}}{\lambda^* - \mu_{jj}^{(0)}} \left[\lambda^* + (\lambda^* - \mu_{jj}^{(0)})\, \eta_{jj}^{(k)}\right]$$

$$g_{ij}^{(k)} = \frac{\alpha_i^{(k)}\, \alpha_j^{(k)}}{\lambda^* - \mu_{jj}^{(0)}}\, \mu_{jj}^{(0)}\, \eta_{ij}^{(k)} \quad (i = 1, 2,\ldots,s,\ i \neq j) \qquad \text{(B.45)}$$

where

$$\eta_{jj}^{(k)} = \sum_{m=s+1}^{n} \frac{\lambda_m}{\lambda_m - \mu_{jj}^{(0)}} \left(\frac{c_{mj}^{(k)}}{\alpha_j^{(k)}} \right)^2$$

$$\eta_{ij}^{(k)} = -\sum_{m=s+1}^{n} \frac{\lambda_m - \lambda^*}{\lambda_m - \mu_{jj}^{(0)}} \left(\frac{c_{mi}^{(k)}}{\alpha_i^{(k)}} \right) \left(\frac{c_{mj}^{(k)}}{\alpha_j^{(k)}} \right) \qquad \text{(B.46)}$$

Since $\bar{d}_j^{(k+1)^T} = (\mu_{1j}^{(k+1)}, \mu_{2j}^{(k+1)}, \ldots, \mu_{sj}^{(k+1)}$ by definition (see Eq. (B.2)), Eqs. (B.39), (B.4), and (B.45) result in

$$\mu_{jj}^{(k+1)} \simeq \lambda^* + (\lambda^* - \mu_{jj}^{(0)})\, \eta_{jj}^{(k)} \qquad (j = 1, 2, \ldots, s)$$

$$\mu_{ij}^{(k+1)} \simeq \mu_{jj}^{(0)}\, \eta_{ij}^{(k)} \qquad (i,j = 1, 2, \ldots, s;\ i \neq j) \qquad \text{(B.47)}$$

Substitution of Eq. (B.43) into Eq. (B.38) results in

$$\Delta c_{ij}^{(k)} = \frac{1}{\lambda_i - \mu_{jj}^{(0)}} \sum_{m=1}^{s} c_{im}^{(k)}\, \mu_{mj}^{(k+1)} - \frac{\lambda_j}{\lambda_i - \mu_{jj}^{(0)}}\, c_{ij}^{(k)}$$

$$= \frac{\lambda^* - \lambda_i}{\lambda_i - \mu_{jj}^{(0)}}\, c_{ij}^{(k)} + \frac{\lambda^*}{\lambda_i - \mu_{jj}^{(0)}} \sum_{m=1}^{s} \left[\delta_{mj}\, \eta_{jj}^{(k)} + \frac{\mu_{mj}^{(0)}}{\lambda^*}\, \eta_{mj}^{(k)} \right]$$

$$= -\, c_{ij}^{(k)} + \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} \left[1 + 0\,(\epsilon^2) \right] c_{ij}^{(k)}$$

$$(i = 1, 2, \ldots, n) \qquad \text{(B.48)}$$

or

$$c_{ij}^{(k+1)} \simeq \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} c_{ij}^{(k)} \qquad (i = 1, 2, \ldots, n) \qquad (B.49)$$

from which, since $\lambda^* = \lambda_1 = \lambda_2 = \ldots = \lambda_n$, it follows that

$$c_{ij}^{(k+1)} \simeq c_{ij}^{(k)} \qquad (i = 1, 2, \ldots, s) \qquad (B.50)$$

Thus,

$$\theta_j^{(k+1)} = \left[\frac{\sum_{i=s+1}^{n} (c_{ij}^{(k+1)})^2}{\sum_{i=1}^{s} (c_{ij}^{(k+1)})^2} \right]^{1/2}$$

$$= \left[\sum_{i=s+1}^{n} \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} \left(\frac{c_{ij}^{(k)}}{\alpha_j^{(k)}} \right)^2 \right]^{1/2}$$

$$\leq h \, \theta_j^{(k)} \qquad (B.51)$$

where $\gamma_j^{(k)}$ is defined in Eq. (B.30), and

$$h = \max_i \left| \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda_i - \mu_{jj}^{(0)}} \right| \qquad (i = s+1, s+2, \ldots, n) \qquad (B.52)$$

To find $\gamma_j^{(k+1)}$, the measure of the error of $\mu_{jj}^{(k+1)}$, Eqs. (B.29) and (B.47) are used, which results in

$$\gamma_j^{(k+1)} = \frac{\lambda^* - \mu_{jj}^{(k+1)}}{\lambda^*}$$

$$\simeq \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda^*} \eta_{jj}^{(k)} \qquad \text{(B.53)}$$

where $\eta_{jj}^{(k)}$ is given in Eq. (B.46). Its absolute value is

$$\left| \eta_{jj}^{(k)} \right| \leq \max_i \left| \frac{\lambda_i}{\lambda_i - \mu_{jj}^{(0)}} \right| \theta_j^{2(k)} \qquad (i = s+1, s+2, \ldots, n) \qquad \text{(B.54)}$$

Therefore, from Eq. (B.53)

$$\gamma_j^{(k+1)} = \zeta \, \theta_j^{2(k)} \qquad \text{(B.55)}$$

where

$$\zeta = \max_i \left| \frac{\lambda_i}{\lambda_i - \mu_{jj}^{(0)}} \right| \cdot \left| \frac{\lambda^* - \mu_{jj}^{(0)}}{\lambda^*} \right| \qquad (i = s+1, s+2, \ldots, n) \qquad \text{(B.56)}$$

From Eqs. (B.55) and (B.51),

$$\gamma_j^{(k+2)} = \zeta \, \theta_j^{2(k+1)}$$

$$= \zeta \, h^2 \, \theta_j^{2(k)}$$

$$= h^2 \, \gamma_j^{(k+1)} \qquad (j = 1, 2, \ldots, s) \qquad \text{(B.57)}$$

Hence, it can be seen from Eqs. (B.5n) and (B.5l) that the multiple eigenvalue and the corresponding eigenvectors converge linearly with errors multiplied by h^2 ($h << 1$) and h respectively in each iteration.

From Eqs. (B.47) and (B.49),

$$\lim_{k\to\infty} \mu_{ij}^{(k)} = \lambda^* \quad \text{for } i = j \qquad (i,j = 1, 2,\ldots,s) \qquad \text{(B.58)}$$
$$= 0 \quad \text{for } i \neq j$$

and

$$\lim_{k\to\infty} c_{ij}^{(k)} = 0 \qquad (i = S+1, s+2,\ldots,n;\ j = 1, 2,\ldots,s) \qquad \text{(B.59)}$$

which shows that as $k\to\infty$, the vectors $\bar{x}_j^{(k)}$ ($j = 1, 2,\ldots,s$) span the subspace of $\bar{x}_j$ ($j = 1, 2,\ldots, s$) whose corresponding eigenvalue is multiple. Thus, the $\bar{x}_j^{(k)}$ ($j = 1, 2,\ldots,s$) themselves are a set of true eigenvectors, orthonormalized with respect to B.

APPENDIX C

THE BASIC THEOREMS ON THE CONSTRAINED STATIONARY-VALUE PROBLEM

Three theorems used for the development of the method for finding multiple or close eigenvalues and the corresponding eigenvectors will be presented. For convenience, two definitions will be given first.

Definition 1

Let S be a set of positive integers p_i ($i = 1,2,\ldots,s$) which are smaller than or equal to n, the order of the matrices A and B of the system $A\bar{x} = \lambda B\bar{x}$, i.e., $S = (p_1, p_2, \ldots, p_s)$. Then, R is defined as the subspace spanned by the s eigenvectors $\bar{x}_i$ ($i \epsilon S$).

Definition 2

If no vector in the subspace R is orthogonal to all vectors $\bar{y}_i$ ($i = 1,2,\ldots,s$) (with respect to B), then the set of the vectors $\bar{y}_i$ ($i = 1,2,\ldots,s$) is said to be an admissible frame with respect to the subspace R.

Theorem 1

With the above definitions, if none of the eigenvalues λ_i ($i \epsilon S$) is equal to any λ_j ($j \notin S$), then among all admissible frames of vectors $\bar{y}_i$ ($i = 1,2,\ldots,s$) a frame which renders w extremum in the following constrained stationary-value problem spans the subspace R, and its stationary value is the sum of the eigenvalues λ_i ($i \epsilon S$):

Find the stationary value of

$$w = \sum_{i=1}^{s} \bar{y}_i^T A \bar{y}_i \qquad (C.1)$$

subject to

$$\bar{y}_i^T B \bar{y}_j = \delta_{ij} \qquad (i,j = 1,2,\ldots,s) \qquad (C.2)$$

where δ_{ij} is the Kronecker delta.

Proof: For convenience, but without loss of generality, the set S = (1,2,...,s n) is taken, that is, R is the subspace spanned by $\bar{x}_i$ (i = 1,2,...,s). Let the vectors $\bar{y}_i$ (i = 1,2,...,s) be expanded in a series of the eigenvectors $\bar{x}_k$ (k = 1,2,...,n):

$$\bar{y}_i = \sum_{k=1}^{n} c_{ki} \bar{x}_k \qquad (k = 1,2,\ldots,n) \qquad (C.3)$$

It will be shown that a solution of Eqs. (C.1) and (C.2) yields

$$c_{ki} = 0 \qquad \text{for } k = s+1,\ s+2,\ldots,n \qquad (C.5)$$

Substitution of Eq. (C.3) into Eqs. (C.1) and (C.2) results in

$$w = \sum_{i=1}^{s} \sum_{i=1}^{n} \lambda_k c_{ki}^2 \qquad (C.6)$$

and

$$\sum_{k=1}^{n} c_{ki}\, c_{kj} = \delta_{ij} \qquad (i,j = 1,2,\ldots,s) \qquad (C.7)$$

Let us use the method of Lagrange multipliers to solve the stationary-value problem of Eqs. (C.6) and (C.7). Introducing the undetermined multipliers μ_{ij} $(i,j = 1,2,\ldots,s)$ and letting $\mu_{ij} = \mu_{ji}$, we have the Lagrangian

$$L = \sum_{i=1}^{s} \sum_{k=1}^{n} \lambda_k c_{ki}^2 - \sum_{i=1}^{s} \sum_{j=1}^{s} \mu_{ij} \left(\sum_{k=1}^{n} c_{ki} c_{kj} - \delta_{ij} \right) \qquad (C.8)$$

Since the first derivatives of L with respect to the unknowns c_{ki} and μ_{ij} should vanish,

$$\frac{\partial L}{\partial c_{ki}} = 2 \left(\lambda_k c_{ki} - \sum_{j=1}^{s} \mu_{ij} c_{kj} \right) = 0 \qquad (C.9)$$

$$\frac{\partial L}{\partial \mu_{ij}} = \sum_{k=1}^{n} c_{ki} c_{kj} - \delta_{ij} = 0 \qquad (C.10)$$

We may write Eqs. (C.9) and (C.10) in matrix form as

$$\Lambda C = C D \qquad (C.11)$$

$$C^T C = I_s \qquad (C.12)$$

where

$$\Lambda = \text{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

$$I_s = \text{unit matrix of order } s$$

and the (k,i)th element of the nxs matrix C is c_{ki} (k = 1,2,...,n; i = 1,2,...,s), and the (i,j)th element of the sxs matrix D is μ_{ij} (i,j = 1,2,...,s). Let the matrix C be partitioned into the two submatrices C_s and C_{n-s}, where C_s is the sxs matrix having the elements of the first s rows of C, and C_{n-s} is the remaining (n-s)xs matrix. Then, Eqs. (C.11) and (C.12) may be written as

$$\Lambda_s C_s = C_s D \tag{C.13}$$

$$\Lambda_{n-s} C_{n-s} = C_{n-s} D \tag{C.14}$$

$$C_s^T C_s + C_{n-s}^T C_{n-s} = I_s \tag{C.15}$$

where

$$\Lambda_s = \text{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_s)$$

$$\Lambda_{n-s} = \text{diag}\,(\lambda_{s+1}, \lambda_{s+2}, \ldots, \lambda_n)$$

Since $\mu_{ij} = \mu_{ji}$ was taken

$$D^T = D \tag{C.16}$$

by which from Eq. (C.13)

$$C_s^T \Lambda_s = D C_s^T \tag{C.17}$$

Postmultiplication of Eq. (C.14) by C and use of Eq. (C.17) leads to

$$\begin{aligned} \Lambda_{n-s} C_{n-s} C_s^T &= C_{n-s} D C_s^T \\ &= C_{n-s} C_s^T \Lambda_s \end{aligned} \tag{C.18}$$

Let

$$U = C_{n-s}\, C_s^T \tag{C.19}$$

Then, Eq. (C.18) yields

$$\lambda_{i+s} u_{ij} = \lambda_j u_{ij} \qquad (i = 1,2,\ldots,n-s;\ j = 1,2,\ldots,s) \tag{C.20}$$

Since

$$U = C_{n-s}\, C_s^T = 0 \tag{C.21}$$

But the set of vectors y $(i = 1,2,\ldots,s)$ is an admissible frame with respect to B, from which it is not difficult to show that

$$\det C_s^T \neq 0 \tag{C.22}$$

From Eqs. (C.21) and (C.22), we obtain

$$C_{n-s} = 0 \tag{C.23}$$

or

$$c_{ki} = 0 \qquad (i = 1,2,\ldots,s;\ k = s+1,s+2,\ldots,n) \tag{C.24}$$

This shows that the subspace spanned by the vectors $\bar{y}_i$ $(i = 1,2,\ldots,s)$ is the subspace of the eigenvectors $\bar{x}_i$ $(i = 1,2,\ldots,s)$, which is to be proved here. Furthermore, from Eq. (C.6) we obtain

$$w = \sum_{i=1}^{s} \sum_{k=1}^{s} \lambda_k c_{ki}^2$$

$$= \sum_{k=1}^{s} \sum_{ki=1}^{s} c_{ki}^2$$

$$= \sum_{k=1}^{s} \lambda_k \qquad (C.25)$$

which implies that the stationary value is the sum of the eigenvalues λ_k ($k = 1,2,\ldots,s$).

Theorem 2

If a frame of s vectors $\tilde{y}_i$ ($i = 1,2,\ldots,s$) which are mutually orthonormal with respect to B spans the subspace R, then Eqs. (C.13), (C.14), and (C.15) are satisfied, i.e., w is stationary.

Proof: Since the vectors $\tilde{y}_i$ ($i = 1,2,\ldots,s$) are in the subspace R, and are orthonormal with respect to B,

$$C_{n-s} = 0$$

and

$$C_s^T C_s = I \quad \text{or} \quad C_s^T = C_s^{-1} \qquad (C.26)$$

Hence, Eqs. (C.14) and (C.15) are satisfied. Furthermore, we have

$$\Lambda_s C_s = (C_s C_s^T)\, \Lambda_s C_s$$

$$= C_s\, (C_s^T\, \Lambda_s C_s) \qquad (C.27)$$

We now define D by $D = C_s^T\, \Lambda_s C_s$, then

$$\Lambda_s C_s = C_s D \qquad (C.28)$$

which is equivalent to Eq. (C.13), i.e., Eq. (C.13) is also satisfied.

Theorem 3

If the s vectors $\bar{y}_i$ (i = 1,2,...,s) span the subspace R of $\bar{x}_i$ ($i \epsilon S$), then the Lagrange multipliers μ_{ij} (i,j = 1,2,...,s) defined in Theorem 1 have the following properties: if the eigenvalues λ_i ($i \epsilon S$) are close together

$$\left| \mu_{ij} \right| << \left| \mu_{ii} \right| \quad \text{for } i \neq j \qquad (C.29)$$

and if the eigenvalues are multiple, i.e., $\lambda^* = \lambda_i$ ($i \epsilon S$)

$$\mu_{ij} = 0 \quad \text{for } i \neq j$$

$$\mu_{ii} = \lambda^* \qquad (C.30)$$

Proof: For convenience, we take the set S = (1,2,...,s).

Then, from Eq. (C.13)

$$D = C_s^T \Lambda_s C_s \tag{C.31}$$

or

$$\mu_{ij} = \sum_{k=1}^{s} \lambda_k c_{ki} c_{kj}$$

$$= \lambda \sum_{ik=1}^{s} c_{ki} c_{kj} + \sum_{k=1}^{s} (\lambda_k - \lambda_i)\, c_{ki} c_{kj} \tag{C.32}$$

From Eq. (C.7)

$$\sum_{k=1}^{s} c_{ki} c_{kj} = \delta_{ij} \qquad (i,j = 1,2,\ldots,s)$$

Thus

$$\mu_{ij} = \sum_{k=1}^{s} (\lambda_k - \lambda_i)\, c_{ki} c_{kj} \qquad \text{for } i \neq j$$

$$\mu_{ii} = \lambda_i + \sum_{k=1}^{s} (\lambda_k - \lambda_i)\, c_{ki}^2 \tag{C.33}$$

If the eigenvalues λ_i $(i = 1,2,\ldots,s)$ are close together, i.e., $| \lambda_k - \lambda_i | << \lambda_i$ $(k \neq i)$, then Eq. (C.33) implies that

$$| \mu_{ij} | << | \mu_{ii} | \qquad \text{for } i \neq j \tag{C.34}$$

Furthermore, if all the eigenvalues λ_i (i = 1,2,...,s) are multiple, i.e., $\lambda^* = \lambda_1 = \lambda_2 =,\ldots, = \lambda_s$, then from Eq. (C.33)

$$\mu_{ij} = 0$$

$$\mu_{ii} = \lambda_i = \lambda^* \qquad (i = 1,2,\ldots,s) \qquad (C.35)$$

TABLE 1. NUMBER OF OPERATIONS FOR EIGENSOLUTIONS

Method	Operation	Calculation	Number of Operations
Proposed Method of Chapter 2	Multiplication	$A - \lambda_j^{(0)} B$	$n\,(m_b + 1)$
	Factorization	$LDU = A - \lambda_j^{(0)} B$	$\frac{1}{2}\, nm_a\,(m_a + 3)$
	Iteration		
	Multiplication	$Ax_j^{(k)}$	$n\,(2m_a + 1)$
		$Bx_j^{(k)}$	$n\,(2m_b + 1)$
		$r_j^{(k)} = Ax_j^{(k)} - \Delta\lambda_j^{(k)} Bx_j^{(k)}$	n
	Factorization	$LDU = F^{(k)}$	$n\,(m_a + 1)$
	Solve Eq. (2.7) for $\Delta x_j^{(k)}$ and $\Delta\lambda_j^{(k)}$		$2n\,(m_a + 1)$
	Total	$N_p = \frac{1}{2}\, pn\,(m_a^2 + 3m_a + 2m_b + 2) + T_p n\,(5m_a + 2m_b + 6)$	

Where

$$F^{(k)} = \begin{bmatrix} A - \lambda_j^{(0)} B & -Bx_j^{(k)} \\ -x_j^{(k)T} B & 0 \end{bmatrix}$$

T_p = Total number of iterations by the proposed method. $T_p > T_r$.

N_p = Total number of operations by the proposed method.

TABLE 1. (Continued)

Method	Operation	Calculation	Number of Operations
Proposed Method of Chapter 3	Multiplication	$A - \mu_{jj}^{(0)} B$	$n(m_b + 1)$
	Factorization	$LDU = A - \mu_{jj}^{(0)} B$	$\frac{1}{2} nm_a (m_a + 3)$
	Iteration		
	Multiplication	$Ay_j^{(k)}$	$n(2m_a + 1)$
	Multiplication	$By_i^{(k)}$ $(i = 1,2,\ldots,s)$	$sn(2m_b + 1)$
	Multiplication	$r_j^{(k)} = Ay_j^{(k)} - \sum_{i=1}^{s} \mu_{ij}^{(k)} By_i^{(k)}$	sn
	Factorization	$LDU = F^{(k)}$	$sn[m_a + \frac{1}{2}(s + 1)]$
	Solve Eq. (3.21) for $\Delta y_j^{(k)}$ and $\Delta d_j^{(k)}$		$n(2m_a + s + 1)$
	Total	$N_p = \frac{1}{2} pn(m_a^2+3m_a+2m_b+2) + T_p n[(s+4)m_a+2sm_b + \frac{1}{2}(s^2+7s+4)]$	

Where

$$F^{(k)} = \begin{bmatrix} A-\mu_{jj}^{(0)}B & -BY^{(k)} \\ -Y^{(k)T}B & 0 \end{bmatrix}$$

$$Y^{(k)} = [y_1^{(k)}, y_2^{(k)}, \ldots, y_s^{(k)}]$$

TABLE 1. (Continued)

Method	Operation	Calculation	Number of Operations
Robinson-Harris Method	Multiplication	$A - \lambda_j^{(k)} B$	$n\,(m_a + 1)$
	Multiplication	$r_j^{(k)} = (A - \lambda_j^{(k)} B)\, x_j^{(k)}$	$n\,(m_a + 1)$
	Multiplication	$Bx_j^{(k)}$	$n\,(m_b + 1)$
	Factorization	$LDU = G^{(k)}$	$\frac{1}{2} nm_a\,(m_a + 5) + n$
	Solve Eq. (2.6) for $\Delta x_j^{(k)}$ and $\Delta\lambda_j^{(k)}$		$2n\,(m_a + 1)$
	Total	$N_r = \frac{1}{2} T_r n\,(m_a^2 + 13m_a + 6_{mb} + 12)$	

Where

$$G^{(k)} = \begin{bmatrix} A - \lambda_j^{(k)} B & -Bx_j^{(k)} \\ -x_j^{(k)T} B & 0 \end{bmatrix}$$

T_r = Total number of iterations by the Robinson-Harris method. $T_r < T_p$.

N_r = Total number of operations by the Robinson-Harris method.

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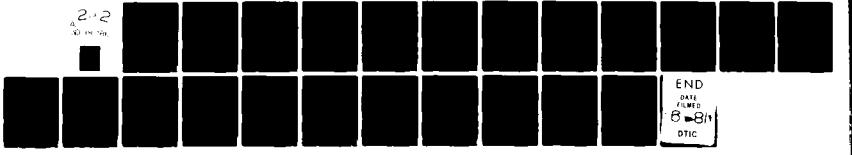

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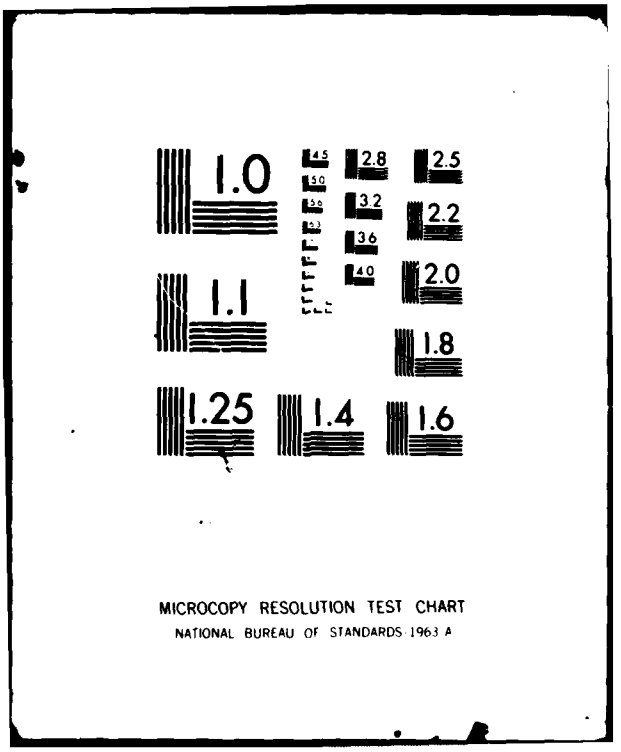
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TABLE 1. (Continued)

Method	Operation	Calculation	Number of Operations
Subspace Iteration Method	Factorization	$LDU = A$	$nm_a\ (m_a + 3)/2$
	Iteration		
	Multiplication	$BX^{(k-1)}$	$qn\ (2m_b + 1)$
	Solve for $Y^{(k)}$	$AY^{(k)} = BX^{(k-1)}$	$qn\ (2m_a + 1)$
	Multiplication	$A^{*(k)} = Y^{(k)^T} BX^{(k-1)}$	$qn\ (q + 1)/2$
	Multiplication	$BY^{(k)}$	$qn\ (2m_b + 1)$
	Multiplication	$B^{*(k)} = Y^{(k)^T} BY^{(k)}$	$qn\ (q + 1)/2$
	Solve for $Z^{(k)}$ and $D^{(k)}$	$A^{*(k)} Z^{(k)} = B^{*(k)} Z^{(k)} D^{(k)}$	$0\ (q^3)$ neglected
	Multiplication	$X^{(k)} = Y^{(k)} Z^{(k)}$	nq^2
	Subtotal		$qn\ (2m_a + 4m_b + 2q + 4)$
	Sturm Sequence Check		
	Multiplication	$A - \lambda_p^{(k)} B$	$n\ (m_b + 1)$
	Factorization	$LDU = A - \lambda_p^{(k)} B$	$nm_a\ (m_a + 3)/2$
	Total	$N_s = T_s qn\ (2m_a) + 4_{mb} + 2q + 4) + n\ (m_a^2 + 3m_a + m_b + 1)$	

Note: $q = \max\ (2p, p+8)$

T_s = Total number of iterations by subspace iteration method.

N_s = Total number of operations by subspace iteration method.

It is assumed that $m_a \geq m_b$.

TABLE 2. EIGENVALUES OF THE PLANE FRAME PROBLEM (DISTINCT ROOTS)

Method of Analysis	Iteration Number	Eigenvalues (1)	(2)	(3)	(4)
Proposed Method	0	0.474744×10^{0}	0.443880×10^{1}	0.132953×10^{2}	0.284745×10^{2}
		(0.36×10^{-2})*	(0.28×10^{-1})	(0.77×10^{-1})	(0.22×10^{0})
	1	0.474744×10^{0}	0.443876×10^{1}	0.132921×10^{2}	0.284091×10^{2}
		(0.44×10^{-5})	(0.45×10^{-3})	(0.38×10^{-2})	(0.27×10^{-1})
	2	0.474744×10^{0}	0.443876×10^{1}	0.132921×10^{2}	0.284091×10^{2}
		(0.82×10^{-13})	(0.27×10^{-9})	(0.17×10^{-6})	(0.18×10^{-3})
	3				0.284091×10^{2}
					(0.19×10^{-5})
	4				0.284091×10^{2}
					(0.23×10^{-7})
Robinson Harris Method	0	0.474744×10^{0}	0.443880×10^{1}	0.132953×10^{2}	0.284745×10^{2}
		(0.36×10^{-2})	(0.28×10^{-1})	(0.77×10^{-1})	(0.22×10^{0})
	1	0.474744×10^{0}	0.443876×10^{1}	0.132921×10^{2}	0.284091×10^{2}
		(0.44×10^{-5})	(0.45×10^{-3})	(0.38×10^{-2})	(0.27×10^{-1})
	2	0.474744×10^{0}	0.443876×10^{1}	0.132921×10^{2}	0.284091×10^{2}
		(0.82×10^{-13})	(0.27×10^{-9})	(0.17×10^{-6})	(0.18×10^{-3})
	3				0.284091×10^{2}
					(0.13×10^{-8})

* : Numbers in parentheses indicate errors in the approximate eigenvectors $x_j^{(k)}$.

TABLE 2. (Continued)

Method of Analysis	Iteration Number	Eigenvalues (1)	(2)	(3)	(4)
Subspace Iteration Method	1	0.476915×10^{0}	0.465927×10^{1}	0.153636×10^{2}	0.369761×10^{2}
	2	0.474744×10^{0} (0.36×10^{-2})*	0.443880×10^{1} (0.28×10^{-1})	0.132953×10^{2} (0.77×10^{-1})	0.284745×10^{2} (0.22×10^{2})
	3	0.474744×10^{0} (0.44×10^{-5})	0.443876×10^{1} (0.44×10^{-3})	0.132921×10^{2} (0.35×10^{-2})	0.284116×10^{2} (0.19×10^{-1})
	4	0.474744×10^{0} (0.11×10^{-7})	0.443876×10^{1} (0.22×10^{-4})	0.132921×10^{2} (0.33×10^{-3})	0.284099×10^{2} (0.48×10^{-2})
	5	0.474744×10^{0} (0.83×10^{-10})	0.443876×10^{1} (0.19×10^{-5})	0.132921×10^{2} (0.90×10^{-4})	0.284094×10^{2} (0.34×10^{-2})
	6	0.474744×10^{0} (0.71×10^{-12})	0.443876×10^{1} (0.16×10^{-6})	0.132921×10^{2} (0.28×10^{-4})	0.284092×10^{2} (0.36×10^{-2})
	7	0.474744×10^{0} (0.11×10^{-13})	0.443876×10^{1} (0.57×10^{-8})	0.132921×10^{2} (0.28×10^{-5})	0.284091×10^{2} (0.11×10^{-2})
	8	0.474744×10^{0} (0.13×10^{-13})	0.443876×10^{1} (0.26×10^{-9})	0.132921×10^{2} (0.28×10^{-6})	0.284091×10^{2} (0.14×10^{-3})
	9	0.474744×10^{0} (0.16×10^{-13})	0.443876×10^{1} (0.17×10^{-10})	0.132921×10^{2} (0.53×10^{-7})	0.284091×10^{2} (0.32×10^{-4})
	10	0.474744×10^{0} (0.13×10^{-13})	0.443876×10^{1} (0.93×10^{-12})	0.132921×10^{2} (0.91×10^{-8})	0.284091×10^{2} (0.99×10^{-5})
	11	0.474744×10^{0} (0.13×10^{-13})	0.443876×10^{1} (0.52×10^{-13})	0.132921×10^{2} (0.12×10^{-8})	0.284091×10^{2} (0.33×10^{-5})
	12	0.474744×10^{0} (0.28×10^{-13})	0.443876×10^{1} (0.50×10^{-13})	0.132921×10^{2} (0.18×10^{-9})	0.284091×10^{2} (0.12×10^{-5})

* : Numbers in parentheses indicate errors in the approximate eigenvectors $x_j^{(k)}$.

TABLE 3. EIGENVALUES OF THE CIRCULAR ARCH PROBLEM (DISTINCT ROOTS)

Method of Analysis	Iteration Number	Eigenvalues/λ_0* (1)	(2)	(3)
Proposed Method	0	0.102714×10^{-2}	0.919516×10^{-2}	0.363073×10^{-1}
	1	0.102640×10^{-2} (0.59×10^{-3})**	0.909467×10^{-2} (0.53×10^{-2})	0.341422×10^{-1} (0.35×10^{-1})
	2	0.102640×10^{-2} (0.26×10^{-8})	0.909467×10^{-2} (0.10×10^{-5})	0.341448×10^{-1} (0.21×10^{-3})
	3		0.909467×10^{-2} (0.10×10^{-8})	0.341448×10^{-1} (0.17×10^{-5})
	4			0.341448×10^{-1} (0.33×10^{-7})
Robinson-Harris Method	0	0.102714×10^{-2}	0.919516×10^{-2}	0.363073×10^{-1}
	1	0.102640×10^{-2} (0.59×10^{-3})	0.909467×10^{-2} (0.53×10^{-2})	0.341422×10^{-1} (0.35×10^{-1})
	2	0.102640×10^{-2} (0.26×10^{-8})	0.909467×10^{-2} (0.10×10^{-5})	0.341448×10^{-1} (0.21×10^{-3})
	3		0.909467×10^{-2} (0.45×10^{-12})	0.341448×10^{-1} (0.20×10^{-8})

* : $\lambda_0 = E/\rho a^2(1-\nu^2)$.

** : Numbers in parentheses indicate errors in the approximate eigenvectors $x_j^{(k)}$.

TABLE 3. (Continued)

Method of Analysis	Iteration Number	Eigenvalues/λ_0* (1)	(2)	(3)
Subspace Iteration Method	1	0.102714×10^{-2}	0.919516×10^{-2}	0.363073×10^{-1}
	2	0.102640×10^{-2} (0.59×10^{-3})**	0.909468×10^{-2} (0.52×10^{-2})	0.341476×10^{-1} (0.32×10^{-1})
	3	0.102640×10^{-2} (0.41×10^{-6})	0.909467×10^{-2} (0.62×10^{-4})	0.341448×10^{-1} (0.26×10^{-2})
	4	0.102640×10^{-2} (0.58×10^{-9})	0.909467×10^{-2} (0.12×10^{-5})	0.341448×10^{-1} (0.23×10^{-3})
	5	0.102640×10^{-2} (0.12×10^{-11})	0.909467×10^{-2} (0.28×10^{-7})	0.341448×10^{-1} (0.21×10^{-4})
	6	0.102640×10^{-2} (0.23×10^{-13})	0.909467×10^{-2} (0.79×10^{-9})	0.341448×10^{-1} (0.19×10^{-5})
	7	0.102640×10^{-2} (0.12×10^{-13})	0.909467×10^{-2} (0.25×10^{-10})	0.341448×10^{-1} (0.17×10^{-6})

* : $\lambda_0 = E/\rho a^2(1-\nu^2)$.

** : Numbers in parentheses indicate errors in the approximate eigenvectors $x_j^{(k)}$.

TABLE 4. EIGENVALUES OF THE SQUARE PLATE PROBLEM (DOUBLE ROOTS)

Method of Analysis	Iteration Number	Eigenvalues/α^* (1)	(2)	(3)	(4)
Proposed Method	0	0.375840×10^{1}	0.230212×10^{2}	0.230212×10^{2}	0.530627×10^{2}
	1	0.375838×10^{1} (0.80×10^{-3})**	0.230121×10^{2} (0.10×10^{-1})	0.230121×10^{2} (0.10×10^{-1})	0.529932×10^{2} (0.21×10^{-1})
	2	0.375838×10^{1} (0.44×10^{-11})	0.230121×10^{2} (0.46×10^{-7})	0.230121×10^{2} (0.46×10^{-7})	0.529932×10^{2} (0.59×10^{-6})
Subspace Iteration Method	1	0.375840×10^{1}	0.230212×10^{2}	0.230212×10^{2}	0.530627×10^{2}
	2	0.375838×10^{1} (0.80×10^{-3})	0.230121×10^{2} (0.10×10^{-1})	0.230121×10^{2} (0.10×10^{-1})	0.529932×10^{2} (0.21×10^{-1})
	3	0.375838×10^{1} (0.65×10^{-6})	0.230121×10^{2} (0.11×10^{-3})	0.230121×10^{2} (0.11×10^{-3})	0.529932×10^{2} (0.43×10^{-3})
	4	0.375838×10^{1} (0.53×10^{-9})	0.230121×10^{2} (0.13×10^{-5})	0.230121×10^{2} (0.13×10^{-5})	0.529932×10^{2} (0.90×10^{-5})
	5	0.375838×10^{1} (0.44×10^{-12})	0.230121×10^{2} (0.15×10^{-7})	0.230121×10^{2} (0.15×10^{-7})	0.529932×10^{2} (0.19×10^{-6})

* : $\alpha = \pi^4 D_e/(a^4\rho)$, where $D_e = Eh^3/12(1 - \nu^2)$.

** : Numbers in parentheses indicate errors in the approximate eigenvectors $y_j^{(k)}$.

TABLE 5. EIGENVALUES OF THE RECTANGULAR PLATE PROBLEM (CLOSE ROOTS)

Method of Analysis	Iteration Number	Eigenvalues/α* (1)	(2)	(3)	(4)
Proposed Method	0	0.368470×10^{1}	0.222957×10^{2}	0.228454×10^{2}	0.520215×10^{2}
	1	0.268468×10^{1} (0.80×10^{-3})	0.222868×10^{2} (0.10×10^{-1})	0.228264×10^{2} (0.10×10^{-1})	0.519522×10^{2} (0.21×10^{-1})
	2	0.368468×10^{1} (0.44×10^{-11})	0.222868×10^{2} (0.47×10^{-7})	0.228364×10^{2} (0.45×10^{-7})	0.519533×10^{2} (0.59×10^{-6})
Subspace Iteration Method	1	0.368470×10^{1}	0.222957×10^{2}	0.228454×10^{2}	0.520215×10^{2}
	2	0.368468×10^{1} (0.80×10^{-3})	0.222868×10^{2} (0.10×10^{-1})	0.228364×10^{2} (0.10×10^{-1})	0.519533×10^{2} (0.21×10^{-1})
	3	0.368468×10^{1} (0.65×10^{-6})	0.222868×10^{2} (0.11×10^{-3})	0.228364×10^{2} (0.11×10^{-3})	0.519533×10^{2} (0.43×10^{-3})
	4	0.368468×10^{1} (0.53×10^{-9})	0.222868×10^{2} (0.13×10^{-5})	0.228364×10^{2} (0.13×10^{-5})	0.519533×10^{2} (0.90×10^{-5})
	5	0.368468×10^{1} (0.46×10^{-12})	0.222868×10^{2} (0.15×10^{-7})	0.228364×10^{2} (0.14×10^{-7})	0.519533×10^{2} (0.19×10^{-6})

* : $\alpha = \pi^4 D_e/(a^4\rho)$, where $D_e = Eh^3/12(1 - \nu^2)$.

** : Numbers in parentheses indicate errors in the approximate eigenvectors $y_j^{(k)}$.

TABLE 6. COMPARISON OF THE TOTAL NUMBER OF OPERATIONS

Problem Type	Input Data					Number of Iterations			Number of Operations			Ratio	
	n	m_a	m_b	p	q	T_p	T_r	T_s	N_p	N_r	N_s	N_r/N_p	N_s/N_p
Frame	330	35	35	4	10	10	9	12	3.50×10^6	4.57×10^6	9.72×10^6	1.31	2.78
Arch	22	4	0	3	5	9	8	7	8.87×10^3	9.77×10^3	1.76×10^4	1.10	1.98
Plate	39	16	16	4	9	8	-	5	1.27×10^5	-	2.20×10^5	-	1.73

Note

n : Order of stiffness and mass matrices

m_a : Average half bandwidth of stiffness matrix

m_b : Average half bandwidth of mass matrix

p : Number of eigenvalues and eigenvectors sought

q : Number of iteration vectors, q = max (2p, p+8)

T_p : Number of iterations by the proposed method

T_r : Number of iterations by the Robinson-Harris method

T_s : Number of iterations by the subspace iteration method

N_p : Total number of operations by the proposed method

N_r : Total number of operations by the Robinson-Harris method

N_s : Total number of operations by the subspace iteration method

TABLE 7. COMPARISON BETWEEN THE THEORETICAL CONVERGENCE RATES FOR EIGENVECTORS AND THE NUMERICAL RESULTS - FRAME PROBLEM (DISTINCT ROOTS)

Method of Analysis	Iteration Number	Eigenvalue Number 1	2	3	4
Proposed Method	1	1.9×10^{-8}	6.0×10^{-7}	4.4×10^{-5}	6.7×10^{-3}
	2				1.1×10^{-2}
	3				1.2×10^{-2}
	Theory	1.3×10^{-8}	1.0×10^{-5}	3.6×10^{-4}	1.2×10^{-2}
Subspace Iteration Method	2	1.2×10^{-3}	1.6×10^{-2}	4.5×10^{-2}	8.6×10^{-2}
	3	2.5×10^{-3}	5.0×10^{-2}	9.4×10^{-2}	2.5×10^{-1}
	4	7.5×10^{-3}	8.7×10^{-2}	2.7×10^{-1}	7.1×10^{-1}
	5	8.6×10^{-3}	8.4×10^{-2}	3.1×10^{-1}	1.1×10^{-0}
	6	1.5×10^{-3}	3.6×10^{-2}	1.0×10^{-1}	3.1×10^{-1}
	7	*	4.6×10^{-2}	1.0×10^{-1}	1.3×10^{-1}
	8	*	6.5×10^{-2}	1.9×10^{-1}	2.3×10^{-1}
	9	*	5.5×10^{-2}	1.7×10^{-1}	3.1×10^{-1}
	10	*	5.6×10^{-2}	1.3×10^{-1}	3.3×10^{-1}
	11	*	*	1.5×10^{-1}	3.6×10^{-1}
	Theory	5.6×10^{-3}	5.2×10^{-2}	1.6×10^{-1}	3.3×10^{-1}

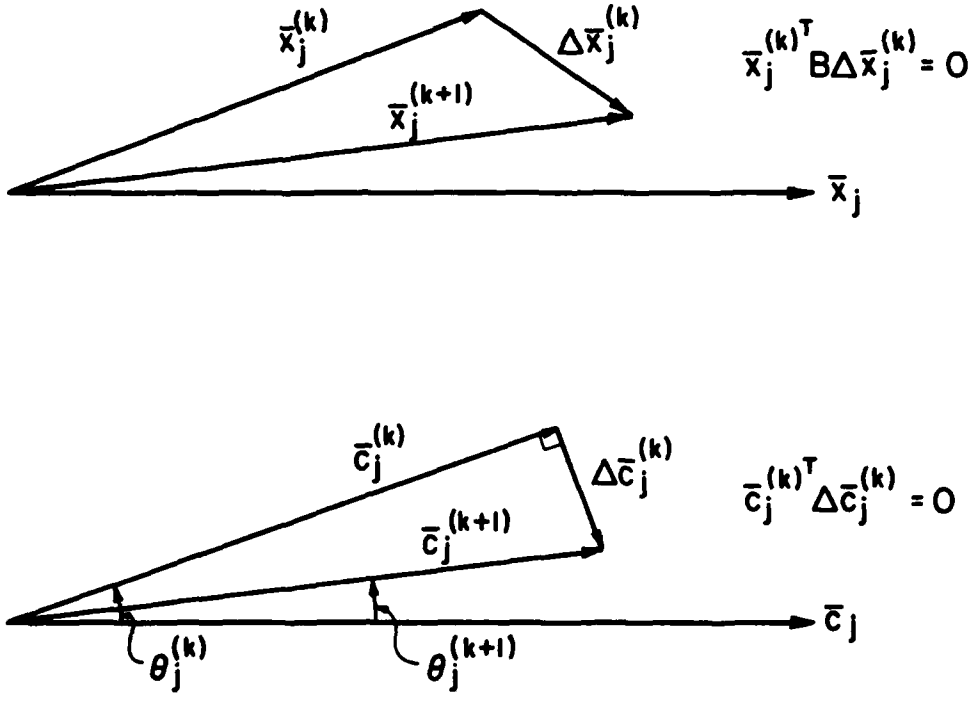
* : Errors too small for comparison because of round-off error.

TABLE 8. COMPARISON BETWEEN THE THEORETICAL CONVERGENCE RATES FOR EIGENVECTORS AND THE NUMERICAL RESULTS - SQUARE PLATE PROBLEM (DOUBLE ROOTS)

Method of Analysis	Iteration Number	Eigenvalue Number 1	2	3	4
Proposed Method	1	5.5×10^{-9}	4.6×10^{-6}	4.6×10^{-6}	2.8×10^{-5}
	Theory	1.0×10^{-6}	4.7×10^{-4}	4.7×10^{-4}	2.3×10^{-3}
Subspace Iteration Method	2	8.1×10^{-4}	1.1×10^{-2}	1.1×10^{-2}	2.0×10^{-2}
	3	8.2×10^{-4}	1.2×10^{-2}	1.2×10^{-2}	2.1×10^{-2}
	4	8.3×10^{-4}	1.2×10^{-2}	1.2×10^{-2}	2.1×10^{-2}
	Theory	1.1×10^{-2}	6.8×10^{-2}	6.8×10^{-2}	1.6×10^{-1}

TABLE 9. NUMERICAL CONVERGENCE RATES FOR EIGENVECTORS - RECTANGULAR PLATE PROBLEM (CLOSE ROOTS)

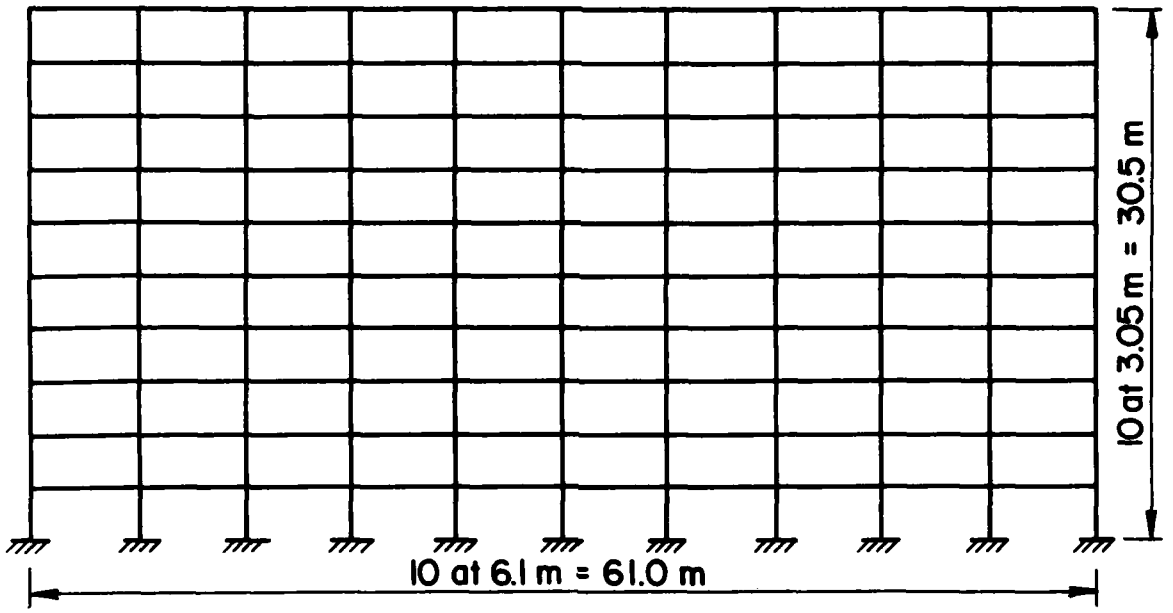
Method of Analysis	Iteration Number	Eigenvalue Number 1	2	3	4
Proposed Method	1	5.5×10^{-9}	4.7×10^{-6}	4.5×10^{-6}	2.8×10^{-5}
Subspace Iteration Method	2	8.1×10^{-4}	1.1×10^{-2}	1.1×10^{-2}	2.0×10^{-2}
	3	8.2×10^{-4}	1.2×10^{-2}	1.2×10^{-2}	2.1×10^{-2}
	4	8.7×10^{-4}	1.2×10^{-2}	1.1×10^{-2}	2.1×10^{-2}
	Theory	1.1×10^{-2}	6.8×10^{-2}	7.0×10^{-2}	1.6×10^{-1}



$$\bar{x}_j^{(k)T} B \Delta\bar{x}_j^{(k)} = 0$$

$$\bar{c}_j^{(k)T} \Delta\bar{c}_j^{(k)} = 0$$

FIG. 1 ESTIMATION OF ERRORS IN APPROXIMATE EIGENVECTORS



For All Beams and Columns

Area of Cross-Section	$A = 2.787 \times 10^{-1}$ m^2
Moment of Inertia of Cross-Section	$I = 8.631 \times 10^{-3}$ m^4
Young's Modulus	$E = 2.068 \times 10^{10}$ Pa
Mass Density	$\rho = 1.602 \times 10^{4}$ kg/m^3

FIG. 2 TEN-STORY, TEN-BAY PLANE FRAME

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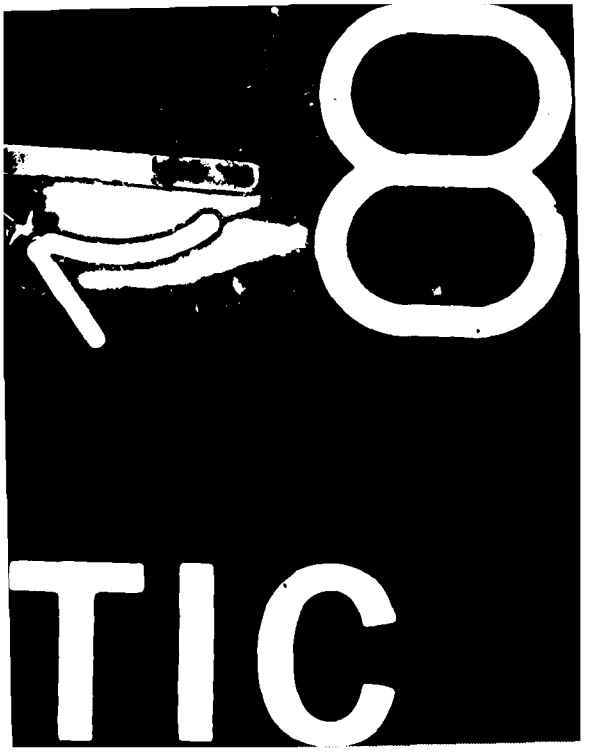
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